April 1992

ISSN 0301-0104

Chemical Physics

A journal devoted to experimental and theoretical research involving problems of both a chemical and a physical nature

MASTER INDEX

VOLUMES 151–160

MARCH 1991–MARCH 1992

Editors
ROBIN M. HOCHSTRASSER/G. LUDWIG HOFACKER

NORTH-HOLLAND

CHEMICAL PHYSICS

A journal devoted to experimental and theoretical research involving problems of both a chemical and a physical nature

EDITORS

ROBIN M. HOCHSTRASSER
Department of Chemistry, University of Pennsylvania,
Philadelphia, PA 19104-6323, USA
FAX 1-215-8988378

G. LUDWIG HOFACKER
Lehrstuhl für Theoretische Chemie, Technische Universität München,
Lichtenbergstrasse 4, 8046 Garching near Munich, Germany
FAX 49-89-32092727

ASSOCIATE EDITOR

DAVID CHANDLER, Department of Chemistry, University of California Berkeley, Berkeley, CA 94720, USA. FAX 1-510-6428369

ADVISORY EDITORIAL BOARD

Australia
R.D. BROWN, Clayton, Victoria
D.P. CRAIG, Canberra
N.S. HUSH, Sydney

Canada
J.C. POLANYI, Toronto

Czechoslovakia
Z. HERMAN, Prague

Denmark
J. LINDERBERG, Aarhus

France
S. LEACH, Orsay
J.-C. LEHMANN, Paris
A. TRAMER, Orsay

Germany
S.F. FISCHER, Garching
W. KAISER, Munich
W. LORENZ, Leipzig
D. MENZEL, Garching
E.W. SCHLAG, Garching
J.P. TOENNIES, Göttingen
H.C. WOLF, Stuttgart
L. ZÜLICKE, Berlin

Israel
J. JORTNER, Tel Aviv
R.D. LEVINE, Jerusalem
M. SHAPIRO, Rehovot

Italy
M. CAPITELLI, Bari
G. ORLANDI, Bologna

Japan
N. MATAGA, Osaka
S. NAGAKURA, Yokohama
K. YOSHIHARA, Okazaki

The Netherlands
J. LOS, Amsterdam
J. REUSS, Nijmegen

Norway
R. MANNE, Bergen

Poland
A. WITKOWSKI, Cracow

Russia
A.I. BURSHTEIN, Novosibirsk
V.S. LETOKHOV, Moscow
R.I. PERSONOV, Troitzk

Sweden
K. SIEGBAHN, Uppsala
E. LINDHOLM, Stockholm

Switzerland
H. FISCHER, Zurich
Hs.H. GÜNTHARD, Zurich
J.P. MAIER, Basel

United Kingdom
A.D. BUCKINGHAM, Cambridge
A. CARRINGTON, Hants
R.N. DIXON, Bristol
D.A. KING, Cambridge
C.J.S.M. SIMPSON, Oxford

USA
A.C. ALBRECHT, Ithaca, NY
H.C. ANDERSEN, Stanford, CA
R. BERSOHN, New York, NY
J.M. DEUTCH, Cambridge, MA
M.D. FAYER, Stanford, CA
G. FLYNN, New York, NY
K.F. FREED, Chicago, IL
W.A. GODDARD III, Pasadena, CA
C.B. HARRIS, Berkeley, CA
E.J. HELLER, Seattle, WA
B. HUDSON, Eugene, OR
M. KLEIN, Philadelphia, PA
Y.T. LEE, Berkeley, CA
W.C. LINEBERGER, Boulder, CO
D.S. McCLURE, Princeton, NJ
J.D. McDONALD, Urbana, IL
W.H. MILLER, Berkeley, CA
T. OKA, Chicago, IL
D.W. OXTOBY, Chicago, IL
C.S. PARMENTER, Bloomington, IN
A. PINES, Berkeley, CA
W. PLUMMER, Philadelphia, PA
W.P. REINHARDT, Philadelphia, PA
G.W. ROBINSON, Lubbock, TX
G.J. SMALL, Ames, IO
J.D. WEEKS, College Park, MD
R.N. ZARE, Stanford, CA
A.H. ZEWAIL, Pasadena, CA
R. ZWANZIG, Bethesda, MD

Yugoslavia
R. BLINC, Ljubljana

Important: please adhere to instructions to authors, to be found on the last pages of each volume.

After acceptance of the paper for publication, further correspondence should be sent to the publishers (Drs. H.A. Arends, Editorial Department, Chemistry & Chemical Engineering Department, P.O. Box 330, 1000 AH Amsterdam, The Netherlands; FAX 31-20-5862459; telex 10704 espom nl; electronic mail X400: C=NL; A=400NET; P=SURF; O=ELSEVIER; S=VONK, I=W or RFC822: W. VONK@ELSEVIER.NL).
Chemical Physics is published semi-monthly. For 1992, 9 volumes, volumes 158–166 (27 issues altogether), have been announced. The subscription price for these volumes is Dfl. 3438.00 (US$ 1877.00). Postage and handling amount to Dfl. 279.00 (US$ 152.50). Therefore the total price is Dfl. 3717.00 (US$ 2029.50). The Dutch guilder price is definitive, dollar prices are for guidance only. Claims for issues not received should be made within three months of publication. If not, they cannot be honoured free of charge.
Subscriptions should be sent to the publisher: Elsevier Science Publishers B.V., Journals Department, P.O. Box 211, 1000 AE Amsterdam, The Netherlands, or to any subscription agent or bookseller.

© Elsevier Science Publishers B.V. All rights reserved. No part of this publication may be reproduced, stored in a retrieval system or transmitted in any form or by any means, electronic, mechanical, photocopying, recording or otherwise, without the prior permission of the publisher, Elsevier Science Publishers B.V., Copyright and Permissions Department, P.O. Box 521, 1000 AM Amsterdam, The Netherlands.
Special regulations for authors. Upon acceptance of an article by the journal, the author(s) will be asked to transfer copyright of the article to the publisher. This transfer will ensure the widest possible dissemination of information.
Submission to this journal of a paper entails the author's irrevocable and exclusive authorization of the publisher to collect any sums or considerations for copying or reproduction payable by third parties (as mentioned in article 17 paragraph 2 of the Dutch Copyright Act of 1912 and in the Royal Decree of June 20, 1974 (S.351) pursuant to article 16b of the Dutch Copyright Act of 1912) and/or to act in or out of Court in connection therewith.
Special regulations for readers in the USA. This journal has been registered with the Copyright Clearance Center, Inc. Consent is given for copying of articles for personal or internal use, or for the personal use of specific clients. This consent is given on the condition that the copier pays through the Center the per-copy fee stated in the code on the first page of each article for copying beyond that permitted by Sections 107 and 108 of the US Copyright Law. The appropriate fee should be forwarded with a copy of the first page of the article to the Copyright Clearance Center, Inc., 27 Congress Street, Salem, MA 01970, USA. If no code appears in an article, the author has not given broad consent to copy and permission to copy must be obtained directly from the author. All articles published prior to 1981 may be copied for a per-copy fee of US$ 2.25, also payable through the Center. This consent does not extend to other kinds of copying, such as for general distribution, resale, advertising and promotion purposes, or for creating new collective works. Special written permission must be obtained from the publisher for such copying.
No responsibility is assumed by the Publisher for any injury and/or damage to persons or property as a matter of products liability, negligence or otherwise, or from any use or operation of any methods, products, instructions or ideas contained in the material herein. Although all advertising material is expected to conform to ethical standards, inclusion in this publication does not constitute a guarantee or endorsement of the quality or value of such product or of the claims made of it by its manufacturer.

Printed in The Netherlands

Published semi-monthly

CHEMICAL PHYSICS

CHEMICAL PHYSICS

A journal devoted to experimental and theoretical research involving problems of both a chemical and a physical nature

EDITORS

ROBIN M. HOCHSTRASSER
Department of Chemistry, University of Pennsylvania,
Philadelphia, PA 19104–6323, USA
FAX 1-215-8988378

G. LUDWIG HOFACKER
Lehrstuhl für Theoretische Chemie, Technische Universität München,
Lichtenbergstrasse 4, 8046 Garching near Munich, Germany
FAX 49-89-32092727

ASSOCIATE EDITOR

DAVID CHANDLER, Department of Chemistry, University of California Berkeley, Berkeley, CA 94720, USA. FAX 1-510-6428369

ADVISORY EDITORIAL BOARD

Australia
R.D. BROWN, Clayton, Victoria
D.P. CRAIG, Canberra
N.S. HUSH, Sydney

Canada
J.C. POLANYI, Toronto

Czechoslovakia
Z. HERMAN, Prague

Denmark
J. LINDERBERG, Aarhus

France
S. LEACH, Orsay
J.-C. LEHMANN, Paris
A. TRAMER, Orsay

Germany
S.F. FISCHER, Garching
W. KAISER, Munich
W. LORENZ, Leipzig
D. MENZEL, Garching
E.W. SCHLAG, Garching
J.P. TOENNIES, Göttingen
H.C. WOLF, Stuttgart
L. ZÜLICKE, Berlin

Israel
J. JORTNER, Tel Aviv
R.D. LEVINE, Jerusalem
M. SHAPIRO, Rehovot

Italy
M. CAPITELLI, Bari
G. ORLANDI, Bologna

Japan
N. MATAGA, Osaka
S. NAGAKURA, Yokohama
K. YOSHIHARA, Okazaki

The Netherlands
J. LOS, Amsterdam
J. REUSS, Nijmegen

Norway
R. MANNE, Bergen

Poland
A. WITKOWSKI, Cracow

Russia
A.I. BURSHTEIN, Novosibirsk
V.S. LETOKHOV, Moscow
R.I. PERSONOV, Troitzk

Sweden
K. SIEGBAHN, Uppsala
E. LINDHOLM, Stockholm

Switzerland
H. FISCHER, Zurich
Hs.H. GÜNTHARD, Zurich
J.P. MAIER, Basel

United Kingdom
A.D. BUCKINGHAM, Cambridge
A. CARRINGTON, Hants
R.N. DIXON, Bristol
D.A. KING, Cambridge
C.J.S.M. SIMPSON, Oxford

USA
A.C. ALBRECHT, Ithaca, NY
H.C. ANDERSEN, Stanford, CA
R. BERSOHN, New York, NY
J.M. DEUTCH, Cambridge, MA
M.D. FAYER, Stanford, CA
G. FLYNN, New York, NY
K.F. FREED, Chicago, IL
W.A. GODDARD III, Pasadena, CA
C.B. HARRIS, Berkeley, CA
E.J. HELLER, Seattle, WA
B. HUDSON, Eugene, OR
M. KLEIN, Philadelphia, PA
Y.T. LEE, Berkeley, CA
W.C. LINEBERGER, Boulder, CO
D.S. McCLURE, Princeton, NJ
J.D. McDONALD, Urbana, IL
W.H. MILLER, Berkeley, CA
T. OKA, Chicago, IL
D.W. OXTOBY, Chicago, IL
C.S. PARMENTER, Bloomington, IN
A. PINES, Berkeley, CA
W. PLUMMER, Philadelphia, PA
W.P. REINHARDT, Philadelphia, PA
G.W. ROBINSON, Lubbock, TX
G.J. SMALL, Ames, IO
J.D. WEEKS, College Park, MD
R.N. ZARE, Stanford, CA
A.H. ZEWAIL, Pasadena, CA
R. ZWANZIG, Bethesda, MD

Yugoslavia
R. BLINC, Ljubljana

CHEMICAL PHYSICS

Editors

ROBIN M. HOCHSTRASSER, Philadelphia

G. LUDWIG HOFACKER, Munich

Associate Editor

DAVID CHANDLER, Berkeley

MASTER INDEX

VOLUMES 151–160

MARCH 1991–MARCH 1992

NORTH-HOLLAND

AMSTERDAM – LONDON – NEW YORK – TOKYO

© 1992 Elsevier Science Publishers B.V. All rights reserved.

No part of this publication may be reproduced, stored in a retrieval system or transmitted in any form or by any means, electronic, mechanical, photocopying, recording or otherwise, without the written permission of the Publisher, Elsevier Science Publishers B.V., Copyright and Permissions Department, P.O. Box 521, 1000 AM Amsterdam, The Netherlands.

Special regulations for authors. *Upon acceptance of an article by the journal, the author(s) will be asked to transfer copyright of the article to the publisher. This transfer will ensure the widest possible dissemination of information.*

Submission to this journal of an article entails the author's irrevocable and exclusive authorization of the publisher to collect any sums or considerations for copying or reproduction payable by third parties (as mentioned in article 17 paragraph 2 of the Dutch Copyright Act of 1912 and in the Royal Decree of June 20, 1974 (S.351) pursuant to article 16b of the Dutch Copyright Act of 1912) and/or to act in or out of Court in connection therewith.

Special regulations for readers in the USA. *This journal has been registered with the Copyright Clearance Center, Inc. Consent is given for copying of articles for personal or internal use, or for the personal use of specific clients. This consent is given on the condition that the copier pays through the Center the per-copy fee stated in the code on the first page of each article for copying beyond that permitted by Sections 107 or 108 of the US Copyright Law. The appropriate fee should be forwarded with a copy of the first page of the article to the Copyright Clearance Center, Inc., 27 Congress Street, Salem, MA 01970, USA. If no code appears in an article, the author has not given broad consent to copy and permission to copy must be obtained directly from the author. All articles published prior to 1981 may be copied for a per-copy fee of US $2.25, also payable through the Center. This consent does not extend to other kinds of copying, such as for general distribution, resale, advertising and promotion purposes, or for creating new collective works. Special written permission must be obtained from the publisher for such copying.*

No responsibility is assumed by the Publisher for any injury and/or damage to persons or property as a matter of products liability, negligence or otherwise, or from any use or operation of any methods, products, instructions or ideas contained in the material herein. Although all advertising material is expected to conform to ethical standards, inclusion in this publication does not constitute a guarantee or endorsement of the quality or value of such product or of the claims made of it by its manufacturer.

Printed on acid-free paper.

PRINTED IN THE NETHERLANDS

Contents

Author index to volumes 151–160 1

Subject index to volumes 151–160 49

METHODS 49

Theoretical 49
Group theory and algebras 49
Classical mechanics 49
Quantized field theory 50
Many body and quasiparticle approaches 50
Coupling schemes and perturbative treatments 51
Relativistic quantum mechanics 51
Transport quantum mechanics 52
Equilibrium statistical mechanics 52
Statistical mechanics of stationary states 52
Non-equilibrium thermodynamic and hydrodynamic theories 53
Ab initio schemes for stationary properties 53
Computational and simulation methods 56
Molecular dynamics and scattering theory 60

Experimental 63
Magnetic resonances 63
Microwave spectroscopy 64
Infrared spectroscopy 65
Raman spectroscopy 65
Visible and UV spectroscopy 66
Fluorescence spectroscopy 68
Photoelectron and Auger spectroscopy 70
X-ray spectroscopy 70
Electron impact spectroscopy 70
Laser methods 71
Picosecond spectroscopy 72
Non-linear optical spectroscopy 73
Synchrotron spectroscopies 73
Coherent optical spectroscopy 74
Optical pumping 74
Multiple resonance spectroscopy 74
Atomic and molecular beam techniques 75
Time-resolved experiments 76
Mass spectrometry 78
X-ray, electron and neutron diffraction 78
Neutron scattering 79
Field emission and field ionization 79
Measurement of macroscopic variables 79

OBJECTS 79

Bulk systems 79
Gases 79
Supersonic beams 80
Liquids neat 81
Liquid mixtures and solutions 81
Crystals 83
  neat 84
  mixed 84
Glasses 85
Liquid crystals 85
Polymers 85
Semiconductors 86
Metals and alloys 86
Thin films 86
Surfaces 86
Low-dimensional materials 87
Dielectrics 87
Plasmas 87
Biological systems 87

Microscopic systems 88
Atoms 88
Molecules (neutral and ionic) 89
  diatomic 90
  small polyatomics 93
  aromatics 96
  other large 97
  polymeric and biological 98
Molecular aggregates 99
  dimers 100
  van der Waals molecules 100
  clusters 100
  complexes 101
Free radicals (including hydronium and muonium) 101
Quasiparticles (including excitons) 102
Defects and impurities 102
Ions and charge carriers 102

PHENOMENA 104

Molecular structure 104
Vibrations and rotations of molecules 105
Electronic structure and states 107
Electric and magnetic properties 111
Spin splittings 112
Optical activity 113
Molecular interactions 113

Spectral bandshapes and intensities 114
Coupling of electronic and nuclear motion 115
Energy transfer processes 116
Molecular photophysical processes 117
Intramolecular dynamics 119
  radiationless transitions 120
  vibrational energy redistribution (including vibrational dissociation) 120
Luminescence spectra, yields and lifetimes 121
Coherence loss processes 122
Non-linear responses (including optical) 122
Reactions (including dissociation) 122
  gas phase 123
  condensed phase 124
  photochemical 125
Tunnelling 126
Electron transfer 127
Positron annihilation 127
Ionization (including Rydberg states) 127
Molecular motion (including diffusive) 129
Fluctuations and noise 130
Collective motion and excitations 130
Surface effects and catalysis 130
Thermodynamic and transport properties 131
Structure of solids and liquids 131
Critical phenomena 132
Phase transitions 132

Author Index to Volumes 151–160

Abascal, J.L.F. and P. Turq, Cluster structure in model electrolyte solutions 153 (1991) 79
Abram, U., see K. Köhler 160 (1992) 281
Abramczyk, H. and J. Kroh, Absorption spectra of a solvated electron in ethers 157 (1991) 373
Abramson, E., see P. Dupré 152 (1991) 293
Abramson, E., see P. Dupré 153 (1991) 539
Achiba, Y., see Y. Luo 153 (1991) 473
Ackermann, J. and H. Hogreve, Adiabatic calculations and properties of the He_2^+ molecular ion 157 (1991) 75
Adam, A.G., Y. Azuma, H. Li, A.J. Merer and C. Thambir, Anomalous structure in the $A^6\Sigma^+$–$X^6\Sigma^+$ transition of MnO caused by interference between two internal hyperfine perturbations 152 (1991) 391
Adamowicz, L., see A. Leś 153 (1991) 409
Adamowicz, L., Theoretical study of optical excitations of linear C_4^- 156 (1991) 387
Adelman, S.A., see F. Patron 152 (1991) 121
Ågren, H., see Y. Luo 153 (1991) 473
Ågren, H., S. Knuts, K.V. Mikkelsen and H.J.Aa. Jensen, Solvatochromatic shifts studied by multi-configuration self-consistent reaction field theory. Application to azabenzenes 159 (1992) 211
Ahmed, A.M., B.F. Campbell, D. Caruso, M.R. Chance, M.D. Chavez, S.H. Courtney, J.M. Friedman, I.E.T. Iben, M.R. Ondrias and M. Yang, Evidence for proximal control of ligand specificity in hemeproteins: absorption and Raman studies of cryogenically trapped photoproducts of ligand bound myoglobins 158 (1991) 329
Åkeby, H. and L.G.M. Pettersson, Core–valence correlation effects on some Cu clusters 155 (1991) 197
Al-Adel, F.F., see P.J. Jewsbury 151 (1991) 103
Albinsson, B., S. Eriksson, R. Lyng and M. Kubista, The electronically excited states of 2-phenylindole 151 (1991) 149
Albrecht, A.C., see A.P. Shreve 154 (1991) 171
Alcamí, M., O. Mó and M. Yáñez, Ab initio molecular orbital treatment of hydroxylamine–X^+–water and hydroxylamine–X^+–ammonia (X=H, Li) clusters 151 (1991) 21
Alekseyev, A.B., V.S. Ivanov, A.M. Pravilov and O.D. Shestakov, Theoretical study of the HeH($B^2\Pi$) fluorescence and predissociation 155 (1991) 173
Alper, J.S., H. Dothe and D.F. Coker, Vibrational structure of the solvated glycine zwitterion 153 (1991) 51
Alsanoosi, A.M. and A.J. Horsewill, Methyl tunnelling in solid diacetyl 160 (1992) 25
Alvira, E., J. Breton, J. Plata and C. Girardet, Chiral discrimination: a model for the interaction between an helicoidal system and an amino acid molecule 155 (1991) 7
Amatore, C., see G. Puccetti 160 (1992) 467
Anderson, M.A. and R.J. Cave, Calculation of excitation energies using quasidegenerate variational perturbation theory and multireference averaged coupled-pair functional theory 154 (1991) 1
André, B., see J.-Y. Moisan 153 (1991) 305
André, B., see J.Y. Moisan 153 (1991) 465

Andrés, J.L., M. Duran, A. Lledós and J. Bertrán, Calculation of the vibrational frequency and line strength versus applied field of carbon monoxide 151 (1991) 37
Andrew, J.J., D.C. McDermott, S.P. Mills and C.J.S.M. Simpson, Near- and non-resonant (VV) energy transfer between molecules dissolved in liquid krypton: a comparison with liquid argon 153 (1991) 247
Angeloni, L., see P. Procacci 154 (1991) 331
Aoyagi, M., see Y. Kubozono 160 (1992) 421
Archirel, P., see N. Levasseur 153 (1991) 387
Arikawa, T., see S. Tsurubuchi 155 (1991) 401
Arrighini, G.P., N. Durante and C. Guidotti, Variational approach to quantum dynamics: a simple application to molecular photodissociation 157 (1991) 365
Ata, M., see Y. Kubozono 160 (1992) 421
Atanasov, M., see D. Reinen 155 (1991) 157
Atkinson, G.H., see D. Blanchard 154 (1991) 155
Augspurger, J.D., see A.I. Jaman 154 (1991) 281
Austin, R.H., M.K. Hong, C. Moser and J. Plombon, Far-infrared perturbation of electron tunneling in reaction centers? 158 (1991) 473
Aziz, R.A., see M.J. Slaman 154 (1991) 33
Azuma, Y., see A.G. Adam 152 (1991) 391

Bagchi, B., see A. Chandra 156 (1991) 323
Bagryanskaya, E.G., see I.A. Shkrob 153 (1991) 427
Bahatt, D., U. Even, E. Shalev, N. Ben-Horin and J. Jortner, Isomer-specific radiative lifetimes of molecular heteroclusters 156 (1991) 223
Bakowies, D. and W. Thiel, Theoretical infrared spectra of large carbon clusters 151 (1991) 309
Balasubramanian, S., see D.G. Lambright 158 (1991) 249
Baldeck, P.L., see M. Pierre 156 (1991) 103
Bañares, L., see A. Heikal 156 (1991) 231
Bancroft, G.M., see J.D. Bozek 158 (1991) 171
Banerjee, A.K., see T. Kundu 156 (1991) 95
Banichevich, A., S.D. Peyerimhoff, B.A. Hess and M.C. van Hemert, Potential curves and predissociation rates for the heavy species HBr^{2+} and DBr^{2+} 154 (1991) 199
Banjavčić, M.P., T.A. Daniels and K.T. Leung, Valence-shell electron momentum distributions of cyclopropane by symmetric noncoplanar (e,2e) spectroscopy 155 (1991) 309
Banjavčić, M.P., see T. Daniels 159 (1992) 289
Baraldi, I., A. Carnevali, F. Momicchioli and G. Ponterini, Theoretical and experimental study on the electronic spectrum and photophysics of Michler's hydrol blue 160 (1992) 85
Barbara, P.F., see W. Jarzeba 152 (1991) 57
Barnett, S.M., N.J. Mason and W.R. Newell, Production of the N_2 ($A\,^3\Sigma_u^+$) metastable state by electron impact dissociative excitation of N_2O 153 (1991) 283
Bartocci, G., see A. Spalletti 160 (1992) 131
Bartolomé, P.H., see T. López Arbeloa 160 (1992) 123
Barzoukas, M., A. Fort, G. Klein, A. Boeglin, C. Serbutoviez, L. Oswald and J.F. Nicoud, Conformational dependence of the quadratic hyperpolarisabilities of a series of push–pull diaryl acetylenes: an experimental and computational investigation 153 (1991) 457
Barzykin, A.V., Spatial distribution of probes in a micelle: effects on the energy transfer time-resolved measurables 155 (1991) 221
Basilevsky, M.V. and G.E. Chudinov, Dynamics of charge transfer chemical reactions in a polar medium within the scope of the Born–Kirkwood–Onsager model 157 (1991) 327
Basilevsky, M.V. and G.E. Chudinov, The configuration interaction theory for charge transfer chemical processes in a polar solvent 157 (1991) 345
Basilevsky, M.V., see G.E. Chudinov 160 (1992) 41
Bates Jr., R.D., see K.L. McNesby 151 (1991) 385
Bates Jr., R.D., see K.L. McNesby 151 (1991) 401
Baum, J., see P. Fan 158 (1991) 295
Baumgärtel, H., see R. Locht 151 (1991) 137
Baumgärtel, H., see R. Locht 155 (1991) 407
Baumgärtel, H., see R. Locht 160 (1992) 477
Bauschlicher Jr., C.W., see M. Rosi 151 (1991) 1
Bauschlicher Jr., C.W., see S.R. Langhoff 153 (1991) 1
Bauschlicher Jr., C.W., see K. Faegri Jr. 153 (1991) 399
Bazhin, N.M., see V.V. Korolev 158 (1991) 129
Beckerle, J.D., M. Casassa, R.R. Cavanagh, E.J. Heilweil and J.C. Stephenson, Sub-picosecond time-resolved IR spectroscopy of the vibrational dynamics of $Rh(CO)_2(acac)$ 160 (1992) 487
Beddard, G.S., see M.G. Hyde 151 (1991) 239
Bednarek, G., see J. Wildt 156 (1991) 497
Beijerinck, H.C.W., see J.P.J. Driessen 155 (1991) 447

Beijersbergen, J.H.M., C.G. de Koster, W.J. van der Zande, P.G. Kistemaker and J. Los, The dissociation dynamics of low lying triplet states in butane and butene molecules 160 (1992) 151
Ben Arfa, M. and M. Tronc, Lowest energy triplet states of group Vb hydrides: NH_3 (ND_3) and PH_3 155 (1991) 143
Bencivenni, L., see F. Ramondo 151 (1991) 179
Bencivenni, L., see F. Ramondo 158 (1991) 41
Benderskii, V.A., V.I. Goldanskii and D.E. Makarov, Low-temperature chemical reactions. Effect of symmetrically coupled vibrations in collinear exchange reactions 154 (1991) 407
Benderskii, V.A., V.I. Goldanskii and D.E. Makarov, Two-dimensional trajectories of tunneling in the symmetric double-well potential 159 (1992) 29
Benetis, N.P., see L. Sjöqvist 156 (1991) 457
Ben-Horin, N., see D. Bahatt 156 (1991) 223
Benjamin, I., L.L. Lee, Y.S. Li, A. Liu and K.R. Wilson, Generalized Langevin model for molecular dynamics of an activated reaction in solution 152 (1991) 1
Berezhkovskii, A.M. and V.Yu. Zitserman, Activated rate processes in the multidimensional case. Consideration of recrossings in the multidimensional Kramers problem with anisotropic friction 157 (1991) 141
Bersuker, I.B., see V.Z. Polinger 159 (1992) 75
Berthier, G., see S. Marguet 160 (1992) 265
Bertrán, J., see J.L. Andrés 151 (1991) 37
Besnainou, S., G. Cardini and D.A. Dows, Molecular dynamics simulation of crystalline imidazole 156 (1991) 71
Biesmans, G., M. Van der Auweraer, C. Cathry, F.C. De Schryver, Y. Yonezawa and T. Sato, On the photo-sensitized injection of electrons into SnO_2 from cyanine dyes incorporated in Langmuir–Blodgett films 160 (1992) 97
Biggs, P., see J. Wildt 159 (1992) 127
Billing, G.D., Quantum-classical reaction path model for chemical reactions. IV. The reaction $Cl^- + CH_3Cl \rightarrow ClCH_3 + Cl^-$ 159 (1992) 109
Bitto, H., see P.R. Willmott 156 (1991) 177
Blaise, P., M. Giry and O. Henri-Rousseau, Driven damped harmonic oscillators perturbed by the parity operator 159 (1992) 169
Blanchard, D., D.A. Gilmore, T.L. Brack, H. Lemaire, D. Hughes and G.H. Atkinson, Picosecond time-resolved absorption and fluorescence in the bacteriorhodopsin photocycle: vibrationally-excited species 154 (1991) 155
Bley, U., P.B. Davies, M. Grantz, T.J. Sears and F. Temps, FIR LMR spectra of FO_2: some classic examples of level anticrossing resonances 152 (1991) 281
Blinc, R., see E. Hadjoudis 156 (1991) 149
Block, D., see M. Pierre 156 (1991) 103
Boeglin, A., see M. Barzoukas 153 (1991) 457
Böhm, M.C. and A. Staib, Material properties of low-dimensional charge-transfer salts. I. Charge fluctuations in systems with stronger electronic correlations 155 (1991) 27
Böhm, M.C., Material properties of low-dimensional charge-transfer salts. II. Mode-softening, Peierls transitions and van Hove singularities 155 (1991) 49
Bohr, F. and M.F. Ruiz-López, Theoretical study of multiple-scattering effects in the X-ray absorption spectra of iron-porphyrins 156 (1991) 55
Boldyrev, A.I. and W. von Niessen, The first ionization potentials of some MH_{k+1}^- and $M_2H_{2k+1}^-$ anions calculated by a Green's function method 155 (1991) 71

Bonamy, J., see S. Temkin 158 (1991) 89
Bonamy, L., see S. Temkin 158 (1991) 89
Bondybey, V.E., see I. Fischer 151 (1991) 295
Bondybey, V.E., see M.F. Cai 155 (1991) 233
Bondybey, V.E., see R. Schlachta 155 (1991) 267
Bonomo, R.P., A.J. Di Bilio and F. Riggi, EPR investigation of chromium(III) complexes: analysis of their frozen solution and magnetically dilute powder spectra 151 (1991) 323
Boom, W., see J.P.J. Driessen 155 (1991) 447
Bosch, E., M. Moreno and J.M. Lluch, A semiclassical simulation for tunneling dynamics of malonaldehyde and hydrogenoxalate anion 159 (1992) 99
Böttcher, R., see K. Köhler 160 (1992) 281
Bouteiller, Y., see H. Hannachi 154 (1991) 23
Boxer, S.G., see D.G. Lambright 158 (1991) 249
Boyd, R.J., see K.V. Darvesh 157 (1991) 99
Bozek, J.D., K.H. Tan, G.M. Bancroft and K.J. Fu, Core level photoionization mass spectroscopy of the fluoromethylsilanes, $Si(CH_3)_xF_{4-x}$ (x=0–4), around the Si 2p ionization edges 158 (1991) 171
Brack, T.L., see D. Blanchard 154 (1991) 155
Bradley, D.D.C., see N. Sato 160 (1992) 299
Braga, M., A. Broo and S. Larsson, Localization and correlation corrections in electronic interactions through single bonded hydrocarbon spacers 156 (1991) 1
Brédas, J.-L., see N. Sato 160 (1992) 299
Bréheret, E., see S. Leach 160 (1992) 451
Breton, J., see E. Alvira 155 (1991) 7
Brion, C.E., see W. Zhang 151 (1991) 343
Brion, C.E., see W. Zhang 151 (1991) 357
Brion, C.E., see W. Zhang 153 (1991) 491
Brion, C.E., see P. Duffy 159 (1992) 347
Brion, C.E., see W. Zhang 160 (1992) 435
Brock, L., see T.C. Devore 155 (1991) 423
Brock, L., see T. Devore 156 (1991) 156
Broo, A., see M. Braga 156 (1991) 1
Brooks, B.R., see P.J. Steinbach 158 (1991) 383
Brosolo, M. and P. Decleva, Variational approach to continuum orbitals in a spline basis: an application to H_2^+ photoionization 159 (1992) 185
Brown, R. and N.A. Efremov, New Monte Carlo simulations of many-particle stochastic dynamics: growth of correlations and local self-ordering during annihilation of like particles 155 (1991) 357
Brühlmann, U., see M. Lombardi 156 (1991) 163
Bruna, P.J. and J.S. Wright, Transition probabilities for the $B\,^1\Delta_g$–$A\,^1\Pi_u$ and $B'\,^1\Sigma_g^+$–$A\,^1\Pi_u$ infrared bands of C_2. An ab initio study 157 (1991) 111
Brunner, H., see R.H. Fritsch 151 (1991) 261
Bubeck, C., A. Kaltbeitzel, A. Grund and M. LeClerc, Resonant degenerate four wave mixing and scaling laws for saturable absorption in thin films of conjugated polymers and Rhodamine 6G 154 (1991) 343
Buchachenko, A.L., see I.A. Shkrob 153 (1991) 443
Buenker, R.J., see L. Chantranupong 154 (1991) 13

Buján-Núñez, M.C., see M.A. López-Quintela 157 (1991) 307
Burlatsky, S.F., G.S. Oshanin and A.A. Ovchinnikov, Kinetics of chemical short-range ordering in liquids and diffusion-controlled reactions 152 (1991) 13
Burri, J. and H. Fischer, Degenerate triplet spin exchange in liquid solution studied by pulse NMR 151 (1991) 279
Burris, J., J. Butler, T. McGee and W. Heaps, Quenching and rotational transfer rates in the $v'=0$ manifold of $OH(A^2\Sigma^+)$ 151 (1991) 233
Burshtein, A.I. and A.A. Zharikov, The probability of non-adiabatic electron transfer as a function of friction 152 (1991) 23
Burshtein, A.I., P.A. Frantsuzov and A.A. Zharikov, Spatial dispersion of electron transfer probability 155 (1991) 91
Bursulaya, B.D., see S.I. Druzhinin 158 (1991) 137
Butler, J., see J. Burris 151 (1991) 233
Butz, T., see P. Mottner 160 (1992) 327
Bzenic, S.A., see S.B. Vrhovac 153 (1991) 233

Caballol, R., see J. Miralles 153 (1991) 25
Cai, L., see S. Lin 160 (1992) 163
Cai, M., see M.B. Partenskii 153 (1991) 125
Cai, M., see M.B. Partenskii 154 (1991) 197
Cai, M.F., C.C. Carter, T.A. Miller and V.E. Bondybey, Laser excitation and resolved emission spectra of supersonically cooled aluminum dimer 155 (1991) 233
Cameron, I.G., see W.T. Sobol 152 (1991) 337
Caminiti, R., see F. Ramondo 151 (1991) 179
Campbell, B.F., see A.M. Ahmed 158 (1991) 329
Caralp, F., see J. Masanet 160 (1992) 383
Cardini, G., see S. Besnainou 156 (1991) 71
Carman, B., see Y. Luo 153 (1991) 473
Carnevali, A., see I. Baraldi 160 (1992) 85
Carter, C.C., see M.F. Cai 155 (1991) 233
Cartwright, D.C., P.J. Hay and S. Trajmar, Estimation of the integral cross section for dissociative excitation of F_2 by electron impact 153 (1991) 219
Caruso, D., see A.M. Ahmed 158 (1991) 329
Casarin, M., G. Granozzi, E. Tondello and A. Vittadini, A theoretical investigation of the hyperfine properties of normal and anomalous muonium in elemental semiconductors: diamond, silicon and germanium 154 (1991) 385
Casarin, M., G. Granozzi, E. Tondello and A. Vittadini, A theoretical investigation of the electronic structure, hyperfine properties and binding energies of muonium centres in cuprous chloride 159 (1992) 365
Casassa, M., see J.D. Beckerle 160 (1992) 487
Casida, M.E., see P. Duffy 159 (1992) 347
Castellucci, E., see A. Tafi 151 (1991) 205
Castro, E.A., see C.G. Diaz 157 (1991) 35
Cathry, C., see G. Biesmans 160 (1992) 97
Cavanagh, R.R., see J.D. Beckerle 160 (1992) 487
Cave, R.J., see M.A. Anderson 154 (1991) 1
Čejchan, A., see V. Špirko 151 (1991) 45
Češpiva, L., see J. Vojtík 156 (1991) 369
Chacón, A., see J.C. Otero 157 (1991) 201
Chaiyapongs, S., see K.P. Sagarik 156 (1991) 439
Chakraborty, T. and M. Chowdhury, Fluorescence excitation spectrum of 1,8-disubstituted naphthalenes in supersonic jet 159 (1992) 439
Champagne, B.B., D.F. Plusquellic, J.F. Pfanstiel, D.W. Pratt, W.M. van Herpen and W.L. Meerts, The trans-stilbene–Ar van der Waals complex. Vibrationally averaged substitution structure in its S_0 and S_1 electronic states 156 (1991) 251
Chance, M.R., see A.M. Ahmed 158 (1991) 329
Chandra, A. and B. Bagchi, Effects of solvent viscoelasticity in the solvation dynamics of an ion in a dense dipolar liquid 156 (1991) 323
Chantranupong, L., G. Hirsch, R.J. Buenker, M. Kimura and M.A. Dillon, Theoretical study of the electronic spectrum of ammonia: generalized oscillator strength calculations for the A–X transition 154 (1991) 13
Chapoulard, D., see S. Guizard 156 (1991) 509
Chapuisat, X., see C. Saint-Espès 159 (1992) 377

Chapuisat, X. and C. Saint-Espès, A weak-mode representation of floppy molecules. II. Kinetic energy and total Hamiltonian matrix 159 (1992) 391
Charutz, D.M. and R.D. Levine, An exact theory of friction for reactive collisions in a solvent using an interaction representation 152 (1991) 31
Charutz, D.M. and R.D. Levine, The dynamics of dressed variables 159 (1992) 321
Chaumet, M., see K. Rościszewski 151 (1991) 159
Chavez, M.D., see A.M. Ahmed 158 (1991) 329
Cheng, Y.D., see Y. Luo 153 (1991) 473
Cherepanova, T.A. and A.V. Stekolnikov, Polyatomic fluids near solid surfaces: a weighted-density-functional approach 154 (1991) 41
Chesnut, D.B. and B.E. Rusiloski, Ab initio calculation of phosphorus NMR chemical shifts in the gauge including atomic orbital method 157 (1991) 105
Chong, D.P., see P. Duffy 159 (1992) 347
Choo, K.Y., see S. Lee 156 (1991) 339
Chowdhury, M., see T. Kundu 156 (1991) 95
Chowdhury, M., see T. Chakraborty 159 (1992) 439
Chu, Z.T., see A. Warshel 158 (1991) 303
Chudinov, G.E., see M.V. Basilevsky 157 (1991) 327
Chudinov, G.E., see M.V. Basilevsky 157 (1991) 345
Chudinov, G.E., D.V. Napolov and M.V. Basilevsky, Quantum-chemical calculations of the hydration energies of organic cations and anions in the framework of a continuum solvent approximation 160 (1992) 41
Chung, W. and S.S. Mak, The two-dimensional electrolytic solution in the hypernetted chain approximation 155 (1991) 19
Clough, S., A.J. Horsewill, M.R. Johnson, M.A. Mohammed and T. Newton, Symmetry breaking in thermally activated NH_4 rotation studied by NMR level crossing spectroscopy 152 (1991) 343
Coker, D.F., see J.S. Alper 153 (1991) 51
Cole, H.B.R. and D.A. Torchia, An NMR study of the backbone dynamics of staphylococcal nuclease in the crystalline state 158 (1991) 271
Colpa, J.P. and F.P. Temme, Structure of MQ-NMR spin spaces under higher $\mathscr{S}_n$- and $(\mathscr{S}_n)\downarrow\mathscr{G}$ symmetries. II. $\Gamma/\tilde{\Gamma}$ $(\mathscr{S}_6)\downarrow\mathscr{O}$ subduced irreps for sixfold spin clusters pertaining to the molecular cage ion, $[BH]_6^{2-}$ 154 (1991) 97
Colpa, J.P., see F.P. Temme 154 (1991) 111
Colpa, J.P. and F.P. Temme, Structure of MQ-NMR spin spaces under higher $\mathscr{S}_n$- and $(\mathscr{S}_n)^{\downarrow}\mathscr{G}$ symmetries. II. $\Gamma/\tilde{\Gamma}$ $(\mathscr{S}_6)^{\downarrow}\mathscr{O}$ subduced irreps for sixfold spin clusters pertaining to the molecular cage ion, $[^{11}BH]_6^{2-}$, Chem. Phys. 154 (1991) 97–110. Erratum 156 (1991) 532
Consalvo, D., see R. Engeln 160 (1992) 427
Cooper, G., see W. Zhang 151 (1991) 343
Cooper, G., see W. Zhang 151 (1991) 357
Cooper, G., see W. Zhang 153 (1991) 491
Correia, N., see M.P. Keane 155 (1991) 379
Cossart-Magos, C., see F. Morlet-Savary 159 (1992) 303
Costes, M., see C. Naulin 153 (1991) 519
Courtney, S.H., see A.M. Ahmed 158 (1991) 329
Crépin, C. and A. Tramer, Electronic spectra and proton transfer in the phenol/$(NH_3)_n$ clusters in argon matrices 156 (1991) 281
Cruciani, G., see A. Spalletti 160 (1992) 131

Cuadros, F. and A. Mulero, Scaling the WCA reference system for two-dimensional Lennard-Jones fluids 156 (1991) 33
Cuadros, F. and A. Mulero, The radial distribution function for two-dimensional Lennard-Jones fluids: computer simulation results 159 (1992) 89
Cuadros, F. and A. Mulero, A validity test of the WCA perturbation theory for two-dimensional Lennard-Jones fluids 160 (1992) 375
Cukrowski, A.S., A.L. Kawczyński, J. Popielawski, W. Stiller and R. Schmidt, Interaction between two chemical reactions in gases. The nonequilibrium effects from the Boltzmann and Fokker–Planck equations within a Lorentz gas model 159 (1992) 39

Da Costa, H.F.M., A.B.F. da Silva, J.R. Mohallem, A.M. Simas and M. Trsic, The generator coordinate Hartree–Fock method for molecular systems. Formalism and first applications to H_2, LiH and Li_2 154 (1991) 379
Daggett, V. and M. Levitt, A molecular dynamics simulation of the C-terminal fragment of the L7/L12 ribosomal protein in solution 158 (1991) 501
Dai, G.H., Q.J. Yan, Y. Wang and Q.S. Liu, Li-doped MgO as catalysts for oxidative coupling of methane: a positron annihilation study 155 (1991) 275
Daniels, T., H. Zhu, M.P. Banjavčić and K.T. Leung, Valence-shell electron momentum distributions and ionization energy spectra of tetramethylsilane by symmetric noncoplanar (e, 2e) spectroscopy 159 (1992) 289
Daniels, T.A., see M.P. Banjavčić 155 (1991) 309
Daragan, V.A. and E.E. Ilyina, Pulsed field gradient NMR for the study of the structure of membrane systems 158 (1991) 105
Darvesh, K.V., P.D. Fricker and R.J. Boyd, Singlet–triplet energy component differences in homonuclear diatomics: a multi-reference configuration interaction study of Hund's rule 157 (1991) 99
Da Silva, A.B.F., see H.F.M. da Costa 154 (1991) 379
Datta, A., see S. Ghoshal 153 (1991) 161
Davies, P.B., see U. Bley 152 (1991) 281
Deakyne, C.A., see M. Shen 151 (1991) 187
Decleva, P., see M. Ohno 156 (1991) 309
Decleva, P., see M. Brosolo 159 (1992) 185
Decleva, P. and M. Ohno, Many-body calculation of the XPS core hole spectra of NiN_2 160 (1992) 341
Decleva, P. and M. Ohno, Many-body calculation of the core hole spectra of PdCO 160 (1992) 353
De Koster, C.G., see J.H.M. Beijersbergen 160 (1992) 151
De Lange, P.J., see B.R. Veenstra 156 (1991) 157
De Lange, P.J., H.Th. Jonkman and K.E. Drabe, Magnetic field dependence of rotationally resolved excitation spectra of the $^1B_{3u}$ 0_0^0 transition of jet-cooled pyrazine 156 (1991) 209
Delhalle, J., see M. Raynaud 153 (1991) 39
Delley, B., see L. Ye 160 (1992) 415
Dennis, T.J., see S. Leach 160 (1992) 451
Denzer, W., see R. Locht 155 (1991) 407
Denzer, W., see R. Locht 160 (1992) 477
De Schryver, F.C., see G. Biesmans 160 (1992) 97
Desouter-Lecomte, M., see F. Remacle 153 (1991) 201
Desprès, A., see S. Leach 160 (1992) 451
Devore, T., L. Brock, R. Kahlscheuer, K. Dulaney and J.L. Gole, On the BiF bond dissociation energy and an evaluation of the BiF red emission band systems, Chem. Phys. 155 (1991) 423–433. Erratum 156 (1991) 156
Devore, T.C., L. Brock, R. Kahlscheuer, K. Dulaney and J.L. Gole, On the BiF bond dissociation energy and an evaluation of the BiF red emission band systems 155 (1991) 423
Dezarnaud, C., M. Tronc and A. Modelli, Shape resonances in low-energy electron transmission and sulfur K-shell photoabsorption spectroscopies: CH_3SH, C_2H_5SH, $(CH_3)_2S$, $(C_2H_5)_2S$, C_6H_5SH, $C_6H_5SCH_3$, CH_3SCN, CH_3NCS, SCl_2 156 (1991) 129
Diaz, C.G., F.M. Fernández and E.A. Castro, Construction of bound-state potential energy curves of diatomic molecules from spectroscopic data 157 (1991) 35
Di Bilio, A.J., see R.P. Bonomo 151 (1991) 323

Diehl, F., see K. Kesper 153 (1991) 511
Diercksen, G.H.F., see V. Špirko 151 (1991) 45
Diercksen, G.H.F. and A.J. Sadlej, Ground state electric properties of NaH 158 (1991) 9
Diercksen, G.H.F., A.J. Sadlej and M. Urban, Electric properties of ionic diatoms: BeO 158 (1991) 19
Dietz, F., see T. Krossner 153 (1991) 63
Dillon, M.A., see L. Chantranupong 154 (1991) 13
Di Martino, V., see F. Ramondo 158 (1991) 41
Dimicoli, I., see F. Morlet-Savary 159 (1992) 303
Doktorov, A.B., see V.A. Morozov 153 (1991) 313
Doktorov, A.B., see V.A. Morozov 153 (1991) 333
Doktorov, A.B., S.A. Mikhailov and P.A. Purtov, Theory of geminate recombination of radical pairs with instantaneously changing spin-Hamiltonian. I. General theory and kinematic approximation 160 (1992) 223
Doktorov, A.B., S.A. Mikhailov and P.A. Purtov, Theory of geminate recombination of radical pairs with instantaneously changing spin-Hamiltonian. II. Method of summation of re-encounter contributions 160 (1992) 239
Domcke, W., see M. Seel 151 (1991) 59
Domcke, W., see A. Staib 156 (1991) 21
Donovan, R.J., see P.J. Jewsbury 151 (1991) 103
Dorfmüller, T., see J. Samios 160 (1992) 33
Dorthe, G., see C. Naulin 153 (1991) 519
Dos Santos, D.A., see F.C. Lavarda 155 (1991) 1
Dothe, H., see J.S. Alper 153 (1991) 51
Dovesi, R., C. Roetti, C. Freyria-Fava, M. Prencipe and V.R. Saunders, On the elastic properties of lithium, sodium and potassium oxide. An ab initio study 156 (1991) 11
Dows, D.A., see S. Besnainou 156 (1991) 71
Drabe, K.E., see P.J. de Lange 156 (1991) 209
Driessen, J.P.J., M.P.I. Manders, F.J.M. van de Weijer, G.J. Sandker, W. Boom, H.C.W. Beijerinck and B.J. Verhaar, Total ionization cross sections for Ne**{$(2p)^5(3p)$; $J=3$}-molecule systems: absolute values and polarization effects 155 (1991) 447
Druzhinin, S.I., B.D. Bursulaya and B.M. Uzhinov, Charged substituents and the effect of their electric field on the electronic spectra of some aminocoumarins 158 (1991) 137
Dubicki, L., see D. Reinen 155 (1991) 117
Duffy, P., M.E. Casida, C.E. Brion and D.P. Chong, Assessment of Gaussian-weighted angular resolution functions in the comparison of quantum-mechanically calculated electron momentum distributions with experiment 159 (1992) 347
Dulaney, K., see T.C. Devore 155 (1991) 423
Dulaney, K., see T. Devore 156 (1991) 156
Dupré, P., R. Jost, M. Lombardi, P.G. Green, E. Abramson and R.W. Field, Anomalous behavior of the anticrossing density as a function of excitation energy in the C_2H_2 molecule 152 (1991) 293
Dupré, P., R. Jost, M. Lombardi, P.G. Green, E. Abramson and R.W. Field, Anomalous behaviour of the anticrossing density as a function of excitation energy in the C_2H_2 molecule, Chem. Phys. 152 (1991) 293. Erratum 153 (1991) 539
Duran, M., see J.L. Andrés 151 (1991) 37
Durante, N., see G.P. Arrighini 157 (1991) 365
Düren, R., R.K.B. Helbing and S. Milošević, Model study of the effect of anisotropy on the differential cross section for atom–molecule scattering: the double rainbows 151 (1991) 287
Dykstra, C.E., see A.I. Jaman 154 (1991) 281

Effenberger, F., see K. Ulrich 154 (1991) 311
Efremov, N.A., see R. Brown 155 (1991) 357
Eggenberger, R., S. Gerber, H. Huber and D. Searles, Ab initio calculation of the second virial coefficient of neon and the potential energy curve of Ne_2 156 (1991) 395
Eilmes, A., see P. Petelenz 155 (1991) 247
Ejeklint, P., see Y. Luo 153 (1991) 473
Ellinger, Y., see M. Raynaud 153 (1991) 39
Engeln, R. and J. Reuss, Methyl torsion in $C_2H_{4-n}(CH_3)_n$, $n=1$ or 2 156 (1991) 215
Engeln, R., D. Consalvo and J. Reuss, Evidence for a gauche minor-conformer of 1,3-butadiene 160 (1992) 427
Englander, J.J., see R.E. McKinnie 158 (1991) 283
Englander, S.W., see R.E. McKinnie 158 (1991) 283
Eriksson, S., see B. Albinsson 151 (1991) 149
Evans, M.W., Circular birefringence and dichroism due to shear stress: optical measurement of non-Newtonian viscosity 154 (1991) 193
Evans, M.W., Theory and simulation of optically induced line shifts in NMR 157 (1991) 1
Even, U., see D. Bahatt 156 (1991) 223

Faegri Jr., K. and C.W. Bauschlicher Jr., Heteronuclear transition metal diatomics: the bonding and electronic structure of ScNi, YNi, ScPd and YPd 153 (1991) 399
Faegri Jr., K., see O. Swang 156 (1991) 379
Fagan, P.J., see J.R.G. Thorne 157 (1991) 401
Fan, P., D. Kominos, D.B. Kitchen, R.M. Levy and J. Baum, Stabilization of α-helical secondary structure during high-temperature molecular-dynamics simulations of α-lactalbumin 158 (1991) 295
Farantos, S.C., see L. Zachilas 154 (1991) 55
Farantos, S.C., The importance of periodic orbits in analysing photodissociation resonances: the O_3 case 159 (1992) 329
Favero, L.B., M.C. Righetti and P.G. Favero, Vibrational energy transfer in the N_2^*–OCS system. Measurements of vibrational populations of the bending manifold in the perturbed steady state by microwave spectroscopy 155 (1991) 107
Favero, P.G., see L.B. Favero 155 (1991) 107
Felder, P., Photodissociation of CF_3I at 248 nm: kinetic energy dependence of the recoil anisotropy 155 (1991) 435
Fenglin, J., see G. Huacai 155 (1991) 345
Feranchuk, I.D., A.P. Ulyanenkov and V.S. Kuz'min, Specific heat from an unsymmetrical double well potential 157 (1991) 61
Fernández, F.M., see C.G. Diaz 157 (1991) 35
Ferrari, L., Heavy ions in mixtures of light gases: Fokker–Planck equation and its solution 153 (1991) 115
Ferretti, A. and A. Lami, Hole pairing on oxygen sites in high-T_c copper–oxide superconductors induced by an effective exchange interaction: a theoretical and numerical investigation on planar lattices 155 (1991) 179
Feulner, P., see R. Treichler 153 (1991) 259
Field, R.W., see P. Dupré 152 (1991) 293
Field, R.W., see P. Dupré 153 (1991) 539
Fielding, H.H., T.P. Softley and F. Merkt, Photoionisation and ZEKE photoelectron spectroscopy of Ar, H_2 and CO_2 using a coherent XUV laser source 155 (1991) 257
Fillaux, F., A. Lautié, J. Tomkinson and G.J. Kearley, Proton transfer dynamics in the hydrogen bond. Inelastic neutron scattering, infrared and Raman spectra of $Na_3H(SO_4)_2$, $K_3H(SO_4)_2$ and $Rb_3H(SO_4)_2$ 154 (1991) 135
Fillaux, F. and J. Tomkinson, Proton-transfer dynamics in the hydrogen bond. Inelastic neutron scattering, infrared and Raman spectra of $KH(CF_3COO)_2$ and $CsH(CF_3COO)_2$ 158 (1991) 113
Fink, E.H., see A.F. Vilesov 153 (1991) 531
Fink, E.H., see J. Wildt 156 (1991) 497
Fink, E.H., see J. Wildt 159 (1992) 127
Fischer, H., see J. Burri 151 (1991) 279
Fischer, I., V.E. Bondybey, P. Rosmus and H.-J. Werner, Theoretical study of the electronic states of BeLi and Be_2^+ 151 (1991) 295
Fleming, G.R., see Y. Hu 158 (1991) 395
Förner, W., The Pariser–Parr–Pople model for trans-polyenes. I. Ab initio and semiempirical study of the bond alternation in trans-butadiene 160 (1992) 173
Förner, W., The Pariser–Parr–Pople model for trans-polyenes. II. Parametrization and ground state dynamics 160 (1992) 189
Fort, A., see M. Barzoukas 153 (1991) 457
Fotakis, C., see E. Patsilinakou 153 (1991) 503

Francisco, J.S. and W.A. Ghoul, Ab initio quantum-chemical study of the unimolecular pyrolysis mechanisms of fluoroformic and chloroformic acid 157 (1991) 89
Francisco, J.S. and I.H. Williams, Structural and spectral consequences of ion-pairing. VI. $BO_2^-Li^+$ and $BO_2^-Na^+$ 160 (1992) 255
Frank, U.E. and W. Hüttner, The diagmagnetic properties of the $\cdot NF_2$ radical by magic doublet rotational Zeeman spectroscopy 152 (1991) 261
Frantsuzov, P.A., see A.I. Burshtein 155 (1991) 91
Fraser, G.T., A.S. Pine, W.A. Kreiner and R.D. Suenram, Optothermal-detected microwave-sideband CO_2-laser spectroscopy of NCH–NH_3 156 (1991) 523
Frauenfelder, H., see R.D. Young 158 (1991) 315
Freed, K.F., see Y. Hu 158 (1991) 395
Freeman, A.J., see L. Ye 160 (1992) 415
Freyria-Fava, C., see R. Dovesi 156 (1991) 11
Fricker, P.D., see K.V. Darvesh 157 (1991) 99
Friedman, H.L., see Y. Zhou 152 (1991) 185
Friedman, H.L., see F.O. Raineri 152 (1991) 201
Friedman, J.M., see A.M. Ahmed 158 (1991) 329
Friend, R.H., see N. Sato 160 (1992) 299
Fritsch, R.H., H. Brunner and K.H. Hausser, Triplet electron–proton cross-polarization by satisfying a modified Hartmann–Hahn condition 151 (1991) 261
Fu, K.J., see J.D. Bozek 158 (1991) 171
Fuke, K., see A. Masaki 158 (1991) 155
Fulde, P., see K. Rościszewski 151 (1991) 159
Furue, H., J.F. LeBlanc, P.D. Pacey and J.M. Whalen, Analytical potential energy surface for methane in terms of interatomic forces 154 (1991) 425

Galasso, V., Ab initio calculations on the one- and two-photon electronic transitions of cyclopentadiene, spirononateraene, 1,4-cyclo-hexadiene, Dewar benzene, norbornadiene, and barrelene 153 (1991) 13
Gale, G.M. and P. Schanne, Time-resolved relaxation of one- and two-vibron states in the rubidium perchlorate crystal 151 (1991) 127
Gale, G.M., see P. Schanne 159 (1992) 1
Galvão, D.S., see F.C. Lavarda 155 (1991) 1
Gamba, Z., The condensed phases of pyrazine: a test of the Williams–Weller intermolecular potential 158 (1991) 59
García de la Vega, J.M. and E. San Fabián, Jahn–Teller effect and dissociation from the ground state of CF_4^+ 151 (1991) 335
Gauyacq, D., see S. Guizard 156 (1991) 509
Gehrke, Ch., R. Mohrschladt, J. Schroeder, J. Troe and P. Vöhringer, Photoisomerization dynamics of diphenylbutadiene in compressed liquid alkanes and in solid environment 152 (1991) 45
Georges, R., see M. Pierre 156 (1991) 103
Gerber, S., see R. Eggenberger 156 (1991) 395
Germann, T.C., see A.I. Jaman 154 (1991) 281
Ghelichkhani, E. and E.R. Grant, On the Jahn–Teller coupling of an orbital triplet with a vibrational doublet 153 (1991) 133
Ghiggino, K.P., see G.D. Scholes 155 (1991) 127
Ghoshal, S. and A. Datta, Doppler-free radio frequency lineshape theory for a three-level system with three allowed transitions in presence of an IR pump 153 (1991) 161
Ghoul, W.A., see J.S. Francisco 157 (1991) 89
Gianturco, F.A., A. Palma and N. Sanna, The He–N_2 interaction revisited: a comparison of measured and computed differential cross sections 158 (1991) 77
Gilmore, D.A., see D. Blanchard 154 (1991) 155
Girardet, C., see E. Alvira 155 (1991) 7
Giro, G. and G. Orlandi, Temperature dependence of the fluorescence spectra of poly-N-vinylcarbazole films from 300 to 550 K: evidence for monomer emission 160 (1992) 145
Giry, M., see P. Blaise 159 (1992) 169
Glasbeek, M., see E. van Oort 152 (1991) 365
Glenewinkel-Meyer, Th., Ch. Ottinger, P. Rosmus and H.-J. Werner, MRCI potential energy functions for the charge transfer reactions $H^+ + HCl\ (X^1\Sigma^+) \rightarrow H + HCl^+\ (X^2\Pi_i, A^2\Sigma^+)$ 152 (1991) 409
Gō, N., see A. Kitao 158 (1991) 447
Gochev, A., see G.E. McManis 152 (1991) 107
Goldanskii, V.I., see V.A. Benderskii 154 (1991) 407
Goldanskii, V.I., see V.A. Benderskii 159 (1992) 29
Gole, J.L., see T.C. Devore 155 (1991) 423
Gole, J.L., see T. Devore 156 (1991) 156
Gondo, Y., see Y. Kubozono 160 (1992) 421
Gorinchoi, N.N., see V.Z. Polinger 159 (1992) 75
Granozzi, G., see M. Casarin 154 (1991) 385
Granozzi, G., see M. Casarin 159 (1992) 365
Grant, E.R., see E. Ghelichkhani 153 (1991) 133
Grantz, M., see U. Bley 152 (1991) 281
Green, P.G., see P. Dupré 152 (1991) 293

Green, P.G., see P. Dupré 153 (1991) 539
Griffiths, W.J. and F.M. Harris, The benzene dication: energies of excited states determined by double-charge-transfer spectroscopy using OH^+ and F^+ projectile ions 157 (1991) 299
Grimm, F.A., T.A. Whitley, P.R. Keller and J.W. Taylor, Absolute partial photoionization cross sections of ethylene 154 (1991) 303
Gropen, O., see O. Swang 156 (1991) 379
Gruber, J.B., see C.A. Morrison 154 (1991) 437
Grund, A., see C. Bubeck 154 (1991) 343
Gryaznov, V.K., see G.L. Gutsev 154 (1991) 291
Guàrdia, E., R. Rey and J.A. Padró, Potential of mean force by constrained molecular dynamics: a sodium chloride ion-pair in water 155 (1991) 187
Guest, J.A., see L.D. Waits 155 (1991) 149
Guidotti, C., see G.P. Arrighini 157 (1991) 365
Guizard, S., N. Shafizadeh, D. Chapoulard, M. Horani and D. Gauyacq, Zeeman effect in the two-photon excitation spectrum of the $C^2\Pi$ state of NO 156 (1991) 509
Gülen, D., Fluorescence depolarization in nonlinear molecular pairs 156 (1991) 123
Gutowsky, H.S., see A.I. Jaman 154 (1991) 281
Gutsev, G.L., V.K. Gryaznov and V.A. Nasluzov, Model potentials in numerical local density functional methods 154 (1991) 291
Gutsev, G.L., The structure and stability of Cl_n^- clusters, $n=2$–7 156 (1991) 427
Gutsev, G.L., The structure and stability of S_2F_{10} and S_2F_{11} and their anions 158 (1991) 33

Ha, T.K., see H.U. Suter 154 (1991) 227
Hadjoudis, E., F. Milia, J. Seliger, V. Zagar and R. Blinc, ^{14}N NQR investigation of some thermochromic and photochromic salicylideneanilines and related compounds 156 (1991) 149
Hagenow, G., see R. Locht 151 (1991) 137
Hagenow, G., see R. Locht 155 (1991) 407
Hald, M. and J.P. Jacobsen, ^{23}Na relaxation in DNA solutions. Influence of intercalation on correlation times and coupling constants 159 (1992) 257
Halvick, P., see M. Monnerville 159 (1992) 227
Hannachi, H., B. Silvi, J.P. Perchard and Y. Bouteiller, Ab initio study of the infrared photoconversion in the water–hydrogen iodide system 154 (1991) 23
Hare, J.P., see S. Leach 160 (1992) 451
Harris, D.L. and B.S. Hudson, Fluorescence and molecular dynamics study of the internal motion of the buried tryptophan in bacteriophage T4 lysozyme: effects of temperature and alteration of nonbonded networks 158 (1991) 353
Harris, F.M., see W.J. Griffiths 157 (1991) 299
Harris, J.M., see X.R. Zhu 157 (1991) 409
Hartke, B. and W. Karrlein, Connecting level statistics and reaction dynamics: mode selective decay of resonant states for HXXH-type molecules 154 (1991) 63
Hausser, K.H., see R.H. Fritsch 151 (1991) 261
Hawlicka, E., see G. Pálinkás 158 (1991) 65
Hay, P.J., see D.C. Cartwright 153 (1991) 219
Hayamizu, K., see S. Hayashi 157 (1991) 381
Hayashi, S. and K. Hayamizu, Spinning-rate depedence of ^{31}P magic-angle-spinning nuclear magnetic resonance spectra in condensed phosphates 157 (1991) 381
Heaps, W., see J. Burris 151 (1991) 233
Heaven, M.C., see M. Macler 151 (1991) 219
Heifets, E.N., The formulae for calculation of g-tensor shifts in third-order perturbation theory 160 (1992) 363
Heikal, A., L. Bañares, D.H. Semmes and A.H. Zewail, Real-time dynamics of vibrational predissociation in anthracene–Ar$_n$ (n=1,2,3) 156 (1991) 231
Heilweil, E.J., see J.D. Beckerle 160 (1992) 487
Heinze, J., see S. Müller 157 (1991) 231
Heinzinger, K., see G. Pálinkás 158 (1991) 65
Helbing, R.K.B., see R. Düren 151 (1991) 287
Hennecke, M. and H.F. Kauffmann, On the fluorescence depolarization in bis-(N-carbazolyl) compounds 157 (1991) 391
Hennico, G., see M. Raynaud 153 (1991) 39
Henri-Rousseau, O., see P. Blaise 159 (1992) 169
Herbich, J. and A. Kapturkiewicz, Radiative and radiationless depopulation of the excited intramolecular charge transfer states: aryl derivatives of aromatic amines 158 (1991) 143
Herman, Z., see J. Vančura 151 (1991) 249
Hermansson, K., From cluster to crystal: ab initio calculations of the OH^- frequency in lithium hydroxide monohydrate 159 (1992) 67
Hess, B.A., see A. Banichevich 154 (1991) 199
Heydtmann, H., see C. Kaupert 156 (1991) 85
Heyes, D.M., Chemical potential, partial enthalpy and partial volume of mixtures by *NPT* molecular dynamics 159 (1992) 149

Hikmet, I., see P. Kowalczyk 160 (1992) 73
Hills, M.E., see C.A. Morrison 154 (1991) 437
Hirata, F., see A. Kitao 158 (1991) 447
Hirayama, S., see A.D. Scully 157 (1991) 253
Hirayama, S., see A.D. Scully 157 (1991) 271
Hirsch, G., see L. Chantranupong 154 (1991) 13
Hitchcock, A.P., see E. Rühl 154 (1991) 323
Hitchman, M.A., see R.G. McDonald 154 (1991) 179
Hitchman, M.A., see D. Reinen 155 (1991) 117
Hochstrasser, R.M., see J.R.G. Thorne 157 (1991) 401
Hochstrasser, R.M., see B. Locke 158 (1991) 409
Hogreve, H., see J. Ackermann 157 (1991) 75
Holmlid, L., see E. Wallin 159 (1992) 313
Hong, M.K., see R.H. Austin 158 (1991) 473
Horani, M., see S. Guizard 156 (1991) 509
Horsewill, A.J., see S. Clough 152 (1991) 343
Horsewill, A.J., see A.M. Alsanoosi 160 (1992) 25
Horwitz, R.J., see L.D. Waits 155 (1991) 149
Hottmann, K., see R. Locht 151 (1991) 137
Hougen, J.T., see P. Uijt de Haag 151 (1991) 371
Hu, Y., G.R. Fleming, K.F. Freed and A. Perico, Theory of long time peptide dynamics: test of various reduced descriptions and role of internal variables 158 (1991) 395
Huacai, G. and J. Fenglin, The phase space moment method for studying intramolecular vibrational energy redistribution 155 (1991) 345
Huber, H., see R. Eggenberger 156 (1991) 395
Huber, J.R., see M. Lombardi 156 (1991) 163
Huber, J.R., see P.R. Willmott 156 (1991) 177
Hudson, B.S., see D.L. Harris 158 (1991) 353
Hughes, D., see D. Blanchard 154 (1991) 155
Hüttner, W., see U.E. Frank 152 (1991) 261
Hwang, J.-K., see A. Warshel 158 (1991) 303
Hyde, M.G. and G.S. Beddard, Picosecond photodissociation and geminate radical recombination in alkane solutions of tetraphenylhydrazine 151 (1991) 239
Hynes, J.T., see G. van der Zwan 152 (1991) 169

Iben, I.E.T., see A.M. Ahmed 158 (1991) 329
Ibuki, T., see W. Zhang 151 (1991) 343
Ibuki, T., see W. Zhang 151 (1991) 357
Ibuki, T., see W. Zhang 153 (1991) 491
Ibuki, T., see W. Zhang 160 (1992) 435
Ida, T., K. Yakushi, H. Kuroda, H. Yamochi and G. Saito, Pressure dependence of the polarized reflectance spectrum of a solid charge-transfer complex, perylene-hexacyanobutadiene (HCBD) 156 (1991) 113
Ida, T., K. Yakushi, H. Kuroda, H. Yamochi and G. Saito, Pressure dependence of the polarized reflectance spectrum of a solid charge-transfer complex, perylene-hexacyanobutadiene (HCBD), Chem. Phys. 156 (1991) 113–122. Erratum 157 (1991) 305
Ilge, H.-D., see K. Ulrich 154 (1991) 311
Ilyina, E.E., see V.A. Daragan 158 (1991) 105
Ito, Y., see I. Tokue 158 (1991) 161
Iturbe, J., see I. Urrecha 154 (1991) 85
Iung, C. and C. Leforestier, A vibrational study of the CD_3H molecule in the curvilinear formulation 155 (1991) 369
Ivanov, V.S., see A.B. Alekseyev 155 (1991) 173

Jackson, R.L., General numerical solution to the time-dependent master equation for non-steady-state reactions: application to the photoinitiated isomerization of cycloheptatriene to toluene 157 (1991) 315
Jacobsen, J.P., see M. Hald 159 (1992) 257
Jaman, A.I., T.C. Germann, H.S. Gutowsky, J.D. Augspurger and C.E. Dykstra, Rotational spectrum and structure of the linear HCN–HCCH dimer 154 (1991) 281
Jarzeba, W., G.C. Walker, A.E. Johnson and P.F. Barbara, Nonexponential solvation dynamics of simple liquids and mixtures 152 (1991) 57
Jelenkovic, B.M., see S.B. Vrhovac 153 (1991) 233
Jensen, H.J.Aa., see H. Ågren 159 (1992) 211
Jewsbury, P.J., K.P. Lawley, T. Ridley, F.F. Al-Adel, P.R.R. Langridge-Smith and R.J. Donovan, Determination of the radiative lifetimes of nine ion-pair states of I_2 151 (1991) 103
Johnson, A.E., see W. Jarzeba 152 (1991) 57
Johnson, J.B., see R.D. Young 158 (1991) 315
Johnson, M.R., see S. Clough 152 (1991) 343
Johr, T., see H. Knöckel 152 (1991) 399
Joly, A.G. and K.A. Nelson, Metal carbonyl photochemistry in organic solvents: femtosecond transient absorption and preliminary resonance Raman spectroscopy 152 (1991) 69
Jonkman, H.Th., see P.J. de Lange 156 (1991) 209
Jönsson, B., see C.E. Woodward 155 (1991) 207
Jordan, P.C., see M.B. Partenskii 153 (1991) 125
Jordan, P.C., see M.B. Partenskii 154 (1991) 197
Jortner, J., see D. Bahatt 156 (1991) 223
Jost, R., see P. Dupré 152 (1991) 293
Jost, R., see P. Dupré 153 (1991) 539
Jurgis, A.J., see E.A. Silinsh 155 (1991) 389
Jutand, A., see G. Puccetti 160 (1992) 467
Juzeliūnas, G., Time-dependent fluorescence depolarization arising from exciton annihilation in confined molecular domains 151 (1991) 169

Kaa, J., see M. Seidl 157 (1991) 279
Kahlscheuer, R., see T.C. Devore 155 (1991) 423
Kahlscheuer, R., see T. Devore 156 (1991) 156
Kaltbeitzel, A., see C. Bubeck 154 (1991) 343
Kapinus, E.I., Friction effect on the mechanism of photochemical redox processes in solutions 152 (1991) 83
Kapturkiewicz, A., see J. Herbich 158 (1991) 143
Karplus, M., see J.E. Straub 158 (1991) 221
Karrlein, W., see B. Hartke 154 (1991) 63
Kashiwagi, H., see Y. Mochizuki 151 (1991) 11
Katalnikov, I.V., see P.P. Levin 154 (1991) 449
Kauffmann, H.F., see M. Hennecke 157 (1991) 391
Kaufman, J.J., see S. Roszak 160 (1992) 1
Kaupert, C., H. Heydtmann and W. Thiel, The vibrational spectra of the monohalogenated cyclopropanes: ab initio calculations and an experimental study of fluorocyclopropane 156 (1991) 85
Kawczyński, A.L., see A.S. Cukrowski 159 (1992) 39
Keane, M.P., A. Naves de Brito, N. Correia, S. Svensson and S. Lunell, Experimental and theoretical study of the N_{1s} and C_{1s} shake-up satellites in pyridine and aniline 155 (1991) 379
Kearley, G.J., see F. Fillaux 154 (1991) 135
Keller, P.R., see F.A. Grimm 154 (1991) 303
Kellö, V. and A.J. Sadlej, Interaction potentials in rare gas–halide ion systems 157 (1991) 123
Kesper, K., F. Diehl, J.G.G. Simon, H. Specht and A. Schweig, Resonant two-photon ionization of phenol in methylene chloride doped solid argon using 248 nm KrF laser and 254 nm Hg lamp radiation, a comparative study. The UV/VIS absorption spectrum of phenol radical cation 153 (1991) 511
Kim, S.K., see E.-K. Lee 157 (1991) 135
Kimura, M., see L. Chantranupong 154 (1991) 13
Kirmse, R., see K. Köhler 160 (1992) 281
Kirski, T., see B. Stein 159 (1992) 269
Kistemaker, P.G., see J.H.M. Beijersbergen 160 (1992) 151
Kitao, A., F. Hirata and N. Gō, The effects of solvent on the conformation and the collective motions of protein: normal mode analysis and molecular dynamics simulations of melittin in water and in vacuum 158 (1991) 447
Kitchen, D.B., see P. Fan 158 (1991) 295
Kivelson, D., see G. Tarjus 152 (1991) 153
Klein, G., see M. Barzoukas 153 (1991) 457
Klimo, V., J. Urban and J. Tiňo, Quasiclassical trajectory study of the effect of reactant rotation on the reaction $B^+ + HD \rightarrow BH^+(BD^+) + D(H)$ 159 (1992) 141
Knöckel, H., T. Johr, H. Richter and E. Tiemann, The influence of the spin–orbit and the hyperfine interaction on the asymptotic behaviour of the $A\,^1\Sigma_u^+$ state of Na_2 152 (1991) 399
Knöckel, H., see H. Richter 157 (1991) 217
Knözinger, H., see P. Mottner 160 (1992) 327
Knuts, S., see H. Ågren 159 (1992) 211
Köhler, K., R. Kirmse, R. Böttcher and U. Abram, Single-crystal EPR and ^{15}N powder ENDOR studies of $[(C_4H_9)_4N][Tc^{VI}NBr_4/Tc^{V}OBr_4]$ 160 (1992) 281
Kokpol, S., see Y.P. Yongyai 156 (1991) 403

Kolenda, J., see B. Stein 159 (1992) 269
Kominos, D., see P. Fan 158 (1991) 295
Kommandeur, J., see B.R. Veenstra 156 (1991) 157
Komorowski, L. and J. Lipiński, Quantumchemical electronegativity and hardness indices for bonded atoms 157 (1991) 45
Korolenko, E.C., see N.V. Shokhirev 154 (1991) 237
Korolev, V.V., D.G. Sushkov and N.M. Bazhin, Diffusion of molecular oxygen in pairs (anthracene–O_2) in glassy matrices 158 (1991) 129
Koutselos, A.D. and E.A. Mason, Generalized Einstein relations for ions in molecular gases 153 (1991) 351
Kowalczyk, P., I. Hikmet and N. Sadeghi, CuBr chemiluminescence from the $Cu^*(^2D_{3/2,5/2}) + Br_2$ reaction 160 (1992) 73
Krausz, E.R., see D. Reinen 155 (1991) 117
Kreile, J., H.-D. Kurland, W. Seibel and A. Schweig, Shape resonances in photoionizations of cyanoacetylene. Experimental and theoretical investigations of the $\tilde{X}\,^2\Pi$, $\tilde{A}\,^2\Sigma$ and $\tilde{B}\,^2\Pi$ ionizations up to a photon energy of 28 eV 155 (1991) 99
Kreiner, W.A., see G.T. Fraser 156 (1991) 523
Kreitzman, S.R., Electron relaxation dynamics of Mu ALCR spectra 152 (1991) 353
Krickemeyer, E., see P. Mottner 160 (1992) 327
Kroes, G.-J. and R.P.H. Rettschnick, Vibrational relaxation of glyoxal in collisions with He and Ar 156 (1991) 293
Kroh, J., see H. Abramczyk 157 (1991) 373
Krossner, T. and F. Dietz, A quantum chemical study on the alternative mechanisms of the thermal cis–trans isomerization of streptocyanines 153 (1991) 63
Kroto, H.W., see S. Leach 160 (1992) 451
Krüger, A., C. Kryschi, L. Valkunas and D. Schmid, Singlet excitation energy transfer in tetracene doped *p*-terphenyl single crystals 157 (1991) 243
Krumschmidt, H. and C. Kryschi, Triplet state IR spectroscopy of aromatic homocycles and heterocycles 154 (1991) 459
Kryschi, C., see H. Krumschmidt 154 (1991) 459
Kryschi, C., see A. Krüger 157 (1991) 243
Kubista, M., see B. Albinsson 151 (1991) 149
Kubozono, Y., T. Miyamoto, M. Aoyagi, M. Ata, Y. Matsuda, Y. Gondo, H. Nakamura and T. Matsuo, The structure and dynamics of 1,3,5-cycloheptatriene and 1,3-cycloheptadiene radical cations in low temperature matrices. An ESR investigation 160 (1992) 421
Kudo, T. and S. Nagase, The structures and stability of the $Si_3H_6^{2+}$ dications. A theoretical study 153 (1991) 379
Kume, H., see I. Tokue 158 (1991) 161
Kundu, T., A.K. Banerjee and M. Chowdhury, Circular dichroism spectrum of gadolinium diglycolate single crystal 156 (1991) 95
Kuntz, P.J., B.I. Niefer and J.J. Sloan, A multisurface classical trajectory study of the dynamics of the reaction $O(^1D_2) + H_2 \rightarrow OH(v', J', \Theta') + H$ using the diatomics in molecules method 151 (1991) 77
Kurland, H.-D., see J. Kreile 155 (1991) 99
Kuroda, H., see T. Ida 156 (1991) 113
Kuroda, H., see T. Ida 157 (1991) 305
Kuwahara, K., see A. Masaki 158 (1991) 155
Kuzmin, V.A., see P.P. Levin 154 (1991) 449

Kuz'min, V.S., see I.D. Feranchuk 157 (1991) 61
Kuznetsov, A.M. and J. Ulstrup, Dissipative relaxation of a low-energy intermediate electronic state in three-level electron transfer 157 (1991) 25

Lacey, A.R., see P. Wormell 160 (1992) 55
Lakhno, V.D. and O.V. Vasil'ev, The solvated electron in an electrolyte solution 153 (1991) 147
Laks, B., see F.C. Lavarda 155 (1991) 1
Lamb, D.C., see R.D. Young 158 (1991) 315
Lambright, D.G., S. Balasubramanian and S.G. Boxer, Protein relaxation dynamics in human myoglobin 158 (1991) 249
Lami, A., see A. Ferretti 155 (1991) 179
Langhoff, S.R., see M. Rosi 151 (1991) 1
Langhoff, S.R., H. Partridge and C.W. Bauschlicher Jr., Theoretical study of the spectroscopy of the alkali oxides LiO, NaO, and KO 153 (1991) 1
Langridge-Smith, P.R.R., see P.J. Jewsbury 151 (1991) 103
Larsson, S., see M. Braga 156 (1991) 1
Lask, G., see R. Schlachta 155 (1991) 267
Lautié, A., see F. Fillaux 154 (1991) 135
Lavarda, F.C., D.A. dos Santos, D.S. Galvão and B. Laks, On the disordered distribution of defects in transpolyacetylene 155 (1991) 1
Lavtchieva, L. and Z. Smedarchina, Generalized golden rule approach to the H-transfer problem. II. Application to a photochemical reaction 160 (1992) 211
Lawley, K.P., see P.J. Jewsbury 151 (1991) 103
Lazzaroni, R., see N. Sato 160 (1992) 299
Leach, S., M. Vervloet, A. Desprès, E. Bréheret, J.P. Hare, T.J. Dennis, H.W. Kroto, R. Taylor and D.R.M. Walton, Electronic spectra and transitions of the fullerene C_{60} 160 (1992) 451
LeBlanc, J.F., see H. Furue 154 (1991) 425
LeClerc, M., see C. Bubeck 154 (1991) 343
Ledoux, I., see G. Puccetti 160 (1992) 467
Lee, D., see S. Lee 156 (1991) 339
Lee, D.J., see E.-K. Lee 157 (1991) 135
Lee, E.-K., D.J. Lee and S.K. Kim, On the critical scattering phenomena of a nonpolar fluid composed of chiral molecules 157 (1991) 135
Lee, J., see S.-B. Zhu 152 (1991) 221
Lee, L.L., see I. Benjamin 152 (1991) 1
Lee, S., M. Yang, K.J. Shin, K.Y. Choo and D. Lee, Theory of diffusion-influenced fluorescence quenching: dependence of the Stern–Volmer curve on light intensity 156 (1991) 339
Leforestier, C., see C. Iung 155 (1991) 369
Lemaire, H., see D. Blanchard 154 (1991) 155
Lerf, A., see P. Mottner 160 (1992) 327
Leroy, J.P., H. Rabitz and R. Wallace, Quantum kinetic energy operator for a group of particles in terms of scalar basic rotational invariant coordinates derived from a generalized Jacobi vector (GJV) description. III. A metric tensors approach 154 (1991) 395
Leś, A. and L. Adamowicz, The correlated molecular electrostatic potential and electric field of 2(1H)-pyrimidone and 2-hydroxypyrimidine 153 (1991) 409
Lesclaux, R., see J. Masanet 160 (1992) 383
Leshina, T.V., see N.V. Shokhirev 154 (1991) 237
Leung, K.T., see M.P. Banjavčić 155 (1991) 309
Leung, K.T., see T. Daniels 159 (1992) 289
Levasseur, N., Ph. Millie, P. Archirel and B. Levy, Bond formation between positively charged species. Non-adiabatic analysis and valence-bond model in the CO^{2+} case 153 (1991) 387

Lever, R., see J.-Y. Moisan 153 (1991) 305
Lever, R., see J.Y. Moisan 153 (1991) 465
Levin, P.P., I.V. Katalnikov and V.A. Kuzmin, Kinetics and magnetic field effect in geminate recombination of triplet radical pairs adsorbed onto porous glass studied by laser flash technique 154 (1991) 449
Levine, R.D., see D.M. Charutz 152 (1991) 31
Levine, R.D., see D.M. Charutz 159 (1992) 321
Levitt, M., see V. Daggett 158 (1991) 501
Levy, B., see N. Levasseur 153 (1991) 387
Levy, R.M., see P. Fan 158 (1991) 295
Ley, L., see J. Masanet 160 (1992) 383
Leyh, B., see R. Locht 155 (1991) 407
Li, H., see A.G. Adam 152 (1991) 391
Li, Y.S., see I. Benjamin 152 (1991) 1
Lian, T., see B. Locke 158 (1991) 409
Liegener, C.-M., The treatment of electron correlation in aperiodic systems. IV. Exciton bands and double ionization potentials 157 (1991) 183
Likhachev, V.N., see G.A. Vinogradov 154 (1991) 367
Lin, M.C., see D.L. Yang 160 (1992) 307
Lin, M.C., see D.L. Yang 160 (1992) 317
Lin, S., X. Yi and L. Cai, Lie algebraic approach to scattering of molecules from a solid surface 160 (1992) 163
Lipiński, J., see L. Komorowski 157 (1991) 45
Lipkin, N., see N. Rom 151 (1991) 199
Liu, A., see I. Benjamin 152 (1991) 1
Liu, Q.S., see G.H. Dai 155 (1991) 275
Lledós, A., see J.L. Andrés 151 (1991) 37
Lluch, J.M., see E. Bosch 159 (1992) 99
Lobo, R.F.M. and A.M.C. Moutinho, A classical study on the vibrational motion of a diatomic molecule in a collisional vibronic excitation 151 (1991) 95
Locht, R., G. Hagenow, K. Hottmann and H. Baumgärtel, Photoionization mass spectrometry of kinetic energy-selected ions. An ion retarding potential difference method applied to NO^+ and O^+ from N_2O 151 (1991) 137
Locht, R., B. Leyh, W. Denzer, G. Hagenow and H. Baumgärtel, The photoionization of ammonia revisited. The vibrational autoionization of NH_3 and its three isotopomers in the 10–12 eV photon energy range 155 (1991) 407
Locht, R., W. Denzer, E. Rühl and H. Baumgärtel, Photoionization mass spectrometry of kinetic energy-selected ions. The translational energy distribution of N^+/N_2 in the inner-shell ionization energy range 160 (1992) 477
Locke, B., T. Lian and R.M. Hochstrasser, Determination of Fe–CO geometry and heme rigidity in carbonmonoxyhemoglobin using femtosecond IR spectroscopy 158 (1991) 409
Lögdlund, M., see N. Sato 160 (1992) 299
Lombardi, M., see P. Dupré 152 (1991) 293
Lombardi, M., see P. Dupré 153 (1991) 539
Lombardi, M., J.P. Pique, U. Brühlmann and J.R. Huber, S_1–T_1 coupling in propynal by level anticrossing spectroscopy 156 (1991) 163
Loncharich, R.J., see P.J. Steinbach 158 (1991) 383

López Arbeloa, F., see T. López Arbeloa 160 (1992) 123
López Arbeloa, I., see T. López Arbeloa 160 (1992) 123
López Arbeloa, T., F. López Arbeloa, P.H. Bartolomé and I. López Arbeloa, On the mechanism of radiationless deactivation of rhodamines 160 (1992) 123
López-Cantarero, E., see J.C. Otero 157 (1991) 201
López-Quintela, M.A. and M.C. Buján-Núñez, Computer simulation of partially diffusion-controlled reactions 157 (1991) 307
Lorquet, J.C., see F. Remacle 153 (1991) 201
Los, J., see J.H.M. Beijersbergen 160 (1992) 151
Loureiro, J., Dissociation rate and N(^{4}S) atom concentrations in a N_2 glow-discharge 157 (1991) 157
Lund, A., see L. Sjöqvist 156 (1991) 457
Lunell, S., see M.P. Keane 155 (1991) 379
Luo, Y., Y.D. Cheng, H. Ågren, R. Maripuu, W. Seibt, L. Öhlund, P. Ejeklint, B. Carman, K.Z. Xing, Y. Achiba and K. Siegbahn, Highly excited states of nitric oxide studied by high-resolution resonance-enhanced multiphoton ionization spectroscopy 153 (1991) 473
Lyng, R., see B. Albinsson 151 (1991) 149

Macler, M. and M.C. Heaven, Spectroscopy and relaxation dynamics of metastable electronically excited states of iodine in rare gas matrices 151 (1991) 219
MacPhail, R.A. and F.C. Monroe, Frequency-dependent solvent friction and torsional damping in liquid 1,2-difluoroethane 152 (1991) 93
Mai, J. and W. von Niessen, The influence of physisorption and the Eley–Rideal mechanism on a surface reaction: $CO+O_2$ 156 (1991) 63
Maier, M., see M. Seidl 157 (1991) 279
Mak, S.S., see W. Chung 155 (1991) 19
Makarov, D.E., see V.A. Benderskii 154 (1991) 407
Makarov, D.E., see V.A. Benderskii 159 (1992) 29
Maki, A.H., see M. Yagi 157 (1991) 209
Makosz, J.J., Experimental determination of the range of interactions of dipole moments in a liquid 155 (1991) 285
Malrieu, J.-P., see J. Miralles 153 (1991) 25
Manders, M.P.I., see J.P.J. Driessen 155 (1991) 447
Marathe, V.R., see K. Nagesha 154 (1991) 125
March, N.H., see A. Nagy 153 (1991) 141
Marcos, J.I., see J.C. Otero 157 (1991) 201
Marguet, S., J.C. Mialocq, P. Millie, G. Berthier and F. Momicchioli, Intramolecular charge transfer and trans–cis isomerization of the DCM styrene dye in polar solvents. A CS INDO MRCI study 160 (1992) 265
Maripuu, R., see Y. Luo 153 (1991) 473
Martin, M.M., P. Plaza and Y.H. Meyer, Transient spectroscopy of triphenylmethane derivatives following subpicosecond irradiation 153 (1991) 297
Maruani, J., see L. Sjöqvist 156 (1991) 457
Masaki, A., T. Ohnuma, K. Kuwahara, H. Umemoto, Y. Wada, F. Misaizu and K. Fuke, Intramultiplet relaxation of $Cd(5^3P_2)$ induced by collisions with N_2 and CO 158 (1991) 155
Masanet, J., F. Caralp, L. Ley and R. Lesclaux, Experimental and theoretical investigation of the reaction $CF_3+NO+M \rightarrow CF_3NO+M$ from 0.5 to 12 Torr and from 253 to 373 K 160 (1992) 383
Masetti, F., see A. Spalletti 160 (1992) 131
Mason, E.A., see A.D. Koutselos 153 (1991) 351
Mason, N.J., see S.M. Barnett 153 (1991) 283
Masuda, A., see I. Tokue 158 (1991) 161
Mathies, H.E., see D. Reinen 155 (1991) 117
Mathur, D., see K. Nagesha 154 (1991) 125
Matsuda, Y., see Y. Kubozono 160 (1992) 421
Matsumoto, A., see A.D. Scully 157 (1991) 253
Matsuo, T., see Y. Kubozono 160 (1992) 421
Matsuoka, S., see S. Tsurubuchi 155 (1991) 401
Matyushov, D.V., Electron transfer induced by liquid defect motion. Exact solution 155 (1991) 331
Mazzucato, U., see A. Spalletti 160 (1992) 131
McCammon, J.A., see J. Shen 158 (1991) 191
McCammon, J.A., see C. Zheng 158 (1991) 261
McDermott, D.C., see J.J. Andrew 153 (1991) 247
McDonald, R.G., R. Stranger, M.A. Hitchman and P.W. Smith, Unusual features in the polarised single crystal electronic spectrum of $(NH_4)_2[V(H_2O)_6](SO_4)_2$: analysis of Fano antiresonance structure and bonding in the $[V(H_2O)_6]^{2+}$ complex 154 (1991) 179

McGee, T., see J. Burris 151 (1991) 233
McKee, M.L., see M.R. Soto 153 (1991) 415
McKinnie, R.E., J.J. Englander and S.W. Englander, Hydrogen-exchange labeling study of the allosteric R-state to T-state equilibrium in methemoglobin 158 (1991) 283
McManis, G.E., A. Gochev and M.J. Weaver, Solvent dynamical effects in electron transfer: the solvent inertial limit and the predicted influence of quantum effects 152 (1991) 107
McNesby, K.L. and R.D. Bates Jr., Secondary heating effects in laser-induced fluorescence experiments 151 (1991) 385
McNesby, K.L. and R.D. Bates Jr., CO_2 laser-induced fluorescence studies of vibrational energy transfer in N_2O 151 (1991) 401
Meath, W.J., see S. Nakai 154 (1991) 349
Meerts, W.L., see P. Uijt de Haag 151 (1991) 371
Meerts, W.L., see E. Zwart 151 (1991) 407
Meerts, W.L. and I. Ozier, Avoided-crossing molecular-beam study of the torsion–rotation energy levels of CH_3CF_3 152 (1991) 241
Meerts, W.L., see P. Uijt de Haag 156 (1991) 197
Meerts, W.L., see B.B. Champagne 156 (1991) 251
Meijers, H.C., see B.R. Veenstra 156 (1991) 157
Meletov, K.P., High pressure study of intermolecular resonance interaction in a naphthalene crystal 154 (1991) 469
Mendaš, I. and P. Milutinović, Trajectory capture rate coefficients for ion–quadrupolar molecule reactions 153 (1991) 73
Menzel, D., see R. Treichler 153 (1991) 259
Merer, A.J., see A.G. Adam 152 (1991) 391
Merkt, F., see H.H. Fielding 155 (1991) 257
Mestdagh, J.M. and J.P. Visticot, Semiempirical electrostatic polarization model of the ionic bonding in alkali and alkaline earth hydroxides and halides 155 (1991) 79
Meyer, Y.H., see M.M. Martin 153 (1991) 297
Mialocq, J.C., see S. Marguet 160 (1992) 265
Mikhailov, S.A., see A.B. Doktorov 160 (1992) 223
Mikhailov, S.A., see A.B. Doktorov 160 (1992) 239
Mikkelsen, K.V., see H. Ågren 159 (1992) 211
Milia, F., see E. Hadjoudis 156 (1991) 149
Miller, T.A., see M.F. Cai 155 (1991) 233
Millie, P., see S. Marguet 160 (1992) 265
Millie, Ph., see N. Levasseur 153 (1991) 387
Mills, S.P., see J.J. Andrew 153 (1991) 247
Milošević, S., see R. Düren 151 (1991) 287
Milutinović, P., see I. Mendaš 153 (1991) 73
Miralles, J., R. Caballol and J.-P. Malrieu, Observable-dedicated molecular orbitals. I. Method and illustrations 153 (1991) 25
Misaizu, F., see A. Masaki 158 (1991) 155
Misurkin, I.A., see A.L. Tchougreeff 153 (1991) 371
Miyamoto, T., see Y. Kubozono 160 (1992) 421
Mó, O., see M. Alcamí 151 (1991) 21
Moc, J., J.M. Rudziński and H. Ratajczak, Comparative study on the structures and energies of the SiX_3, GeX_3 and SnX_3 series of radicals (X=H, F, Cl) 159 (1992) 197

Mochizuki, Y., K. Tanaka and H. Kashiwagi, Electronic structure of linear form of OCuO 151 (1991) 11
Modelli, A., see C. Dezarnaud 156 (1991) 129
Mohallem, J.R., see H.F.M. da Costa 154 (1991) 379
Mohammed, M.A., see S. Clough 152 (1991) 343
Mohrschladt, R., see Ch. Gehrke 152 (1991) 45
Moisan, J.-Y., B. André and R. Lever, Xerographic dark discharge of PVK:TNF photoconductive material 153 (1991) 305
Moisan, J.Y., B. André, R. Lever and C. Servens, Xerographic discharge of organic thermoplastic material 153 (1991) 465
Moiseyev, N., see N. Rom 151 (1991) 199
Momicchioli, F., see G. Ponterini 151 (1991) 111
Momicchioli, F., see I. Baraldi 160 (1992) 85
Momicchioli, F., see S. Marguet 160 (1992) 265
Monnerville, M., P. Halvick and J.C. Rayez, Time-dependent calculation of the energy resolved state-to-state transition probabilities for three-atom exchange reactions 159 (1992) 227
Monroe, F.C., see R.A. MacPhail 152 (1991) 93
Moreno, M., see E. Bosch 159 (1992) 99
Morlet-Savary, F., I. Dimicoli, C. Cossart-Magos and J.E. Parkin, Characterization of the $\tilde{B}\leftarrow\tilde{X}$ transition of the chlorobenzene cation prepared in non-equilibrium rotational population distributions by resonance enhanced multiphoton ionization 159 (1992) 303
Moro, G.J., Master equation for site distributions describing barrier crossing in the presence of anisotropic diffusion 159 (1992) 421
Morozov, V.A. and A.B. Doktorov, Theory of multiquantum optically detected ESR spectra of radical pairs. I. General theory. Resonances in parallel radio-frequency field 153 (1991) 313
Morozov, V.A. and A.B. Doktorov, Theory of multiquantum optically detected ESR spectra of radical pairs. II. Resonances in perpendicular radio-frequency field 153 (1991) 333
Morrison, C.A., J.B. Gruber and M.E. Hills, Energy levels of Cr^{3+} ions in C_{3i} sites of $Y_3Al_5O_{12}$ 154 (1991) 437
Moser, C., see R.H. Austin 158 (1991) 473
Motohashi, K., see S. Tsurubuchi 155 (1991) 401
Mottner, P., A. Lerf, T. Butz, H. Knözinger, A. Müller, V. Wittneben and E. Krickemeyer, Nuclear quadrupole interaction of $^{99}Mo(\beta^-)^{99}Tc$ in various molybdenum sulfur cluster compounds and thermal decomposition products of $(NH_4)_2[Mo_3S(S_2)_6]\cdot nH_2O$ (n= 0–2) 160 (1992) 327
Moutinho, A.M.C., see R.F.M. Lobo 151 (1991) 95
Mucha, D., see P. Petelenz 154 (1991) 145
Mulero, A., see F. Cuadros 156 (1991) 33
Mulero, A., see F. Cuadros 159 (1992) 89
Mulero, A., see F. Cuadros 160 (1992) 375
Müller, A., see P. Mottner 160 (1992) 327
Müller, S. and J. Heinze, Fluorescence analysis of two new TICT systems: 10-cyano-9,9′-bianthryl (CBA) and 10,10′-dicyano-9,9′-bianthryl (DCBA) 157 (1991) 231

Nagase, S., see T. Kudo 153 (1991) 379
Nagesha, K., V.R. Marathe and D. Mathur, An experimental and theoretical study of SF^{q+} ($q=1$–3) ions 154 (1991) 125
Nagy, A. and N.H. March, Relation between total energy and sum of orbital energies for neutral atoms 153 (1991) 141
Nakai, S. and W.J. Meath, On the validity of the RWA for steady state and temporal populations of molecular states involved in IR multi-photon excitations 154 (1991) 349
Nakamura, H., see Y. Kubozono 160 (1992) 421
Nakashima, K., see T. Ogawa 156 (1991) 465
Nakashima, K., see T. Ogawa 156 (1991) 473
Napolov, D.V., see G.E. Chudinov 160 (1992) 41
Nasluzov, V.A., see G.L. Gutsev 154 (1991) 291
Naulin, C., M. Costes and G. Dorthe, The $C(^3P_J)+NO(X^2\Pi_r)\rightarrow CN(X^2\Sigma^+)+O(^3P_J)$ reaction dynamics studied at 0.06 and 0.23 eV relative translational energy in pulsed crossed supersonic molecular beams 153 (1991) 519
Naves de Brito, A., see M.P. Keane 155 (1991) 379
Nelander, B., A matrix isolation study of the water–formaldehyde complex. The far-infrared region 159 (1992) 281
Nelson, K.A., see A.G. Joly 152 (1991) 69
Newell, W.R., see S.M. Barnett 153 (1991) 283
Newton, T., see S. Clough 152 (1991) 343
Nicoud, J.F., see M. Barzoukas 153 (1991) 457
Niefer, B.I., see P.J. Kuntz 151 (1991) 77
Nienhaus, G.U., see R.D. Young 158 (1991) 315
Noid, D.W., see B.G. Sumpter 160 (1992) 393

O, H.-K., see M.-C. Su 156 (1991) 261
Ochi, N. and S. Tsuchiya, Rovibronic level structure of electronically excited acetylene ($\tilde{A}\,^1A_u$) in a supersonic jet as studied by laser-induced fluorescence and Zeeman quantum beat spectroscopy 152 (1991) 319
Oddershede, J., see S.P.A. Sauer 153 (1991) 189
Ogawa, T., T. Tsuboi and K. Nakashima, Dissociation of aliphatic hydrocarbons excited by electrons: translational energy distributions of the excited hydrogen atom 156 (1991) 465
Ogawa, T., M. Tsukada and K. Nakashima, Dissociation of hydrogen sulfide in e–H_2S collisions: translational energy distribution of $H^*(n=4)$ 156 (1991) 473
Ogryzlo, E.A., see Z.H. Walker 153 (1991) 483
Öhlund, L., see Y. Luo 153 (1991) 473
Ohno, M. and P. Decleva, Many-body calculations of the core hole spectra of NiCO 156 (1991) 309
Ohno, M., W. von Niessen and J. Schüle, Many-body calculation of the valence photoemission spectrum of ferrocene 158 (1991) 1
Ohno, M., see P. Decleva 160 (1992) 341
Ohno, M., see P. Decleva 160 (1992) 353
Ohnuma, T., see A. Masaki 158 (1991) 155
Okamoto, H., Effects of homogeneous and inhomogeneous broadening mechanisms and molecular rearrangement dynamics on frequency resolved and time resolved coherent Raman intensities 155 (1991) 291
Okamoto, M., see A.D. Scully 157 (1991) 271
Ondrias, M.R., see A.M. Ahmed 158 (1991) 329
Orlandi, G., see G. Giro 160 (1992) 145
Oshanin, G.S., see S.F. Burlatsky 152 (1991) 13
Oswald, L., see M. Barzoukas 153 (1991) 457
Otero, J.C., J.I. Marcos, E. López-Cantarero and A. Chacón, Ring-puckering and internal rotation barriers in N,N′-dimethylethyleneurea 157 (1991) 201
Ottinger, Ch., see Th. Glenewinkel-Meyer 152 (1991) 409
Ovchinnikov, A.A., see S.F. Burlatsky 152 (1991) 13
Ovchinnikov, A.A., see G.A. Vinogradov 154 (1991) 367
Owens, T.G., see A.P. Shreve 154 (1991) 171
Ozier, I., see W.L. Meerts 152 (1991) 241

Pacey, P.D., see H. Furue 154 (1991) 425
Padró, J.A., see E. Guàrdia 155 (1991) 187
Page, M., see M.R. Soto 153 (1991) 415
Paidarová, I., see J. Vojtík 156 (1991) 369
Paidarová, I., see J. Vojtík 157 (1991) 67
Pálinkás, G., E. Hawlicka and K. Heinzinger, Molecular dynamics simulations of water–methanol mixtures 158 (1991) 65
Palma, A., see F.A. Gianturco 158 (1991) 77
Palmer, M.H., see I.C. Walker 153 (1991) 169
Palmer, M.H. and I.C. Walker, The electronic states of the azines. V. Pyridazine, studied by VUV absorption, near threshold electron energy-loss spectroscopy and ab initio multi-reference configuration interaction calculations 157 (1991) 187
Parkin, J.E., see F. Morlet-Savary 159 (1992) 303
Parmenter, C.S., see M.-C. Su 156 (1991) 261
Parsegian, V.A., see R. Podgornik 154 (1991) 477
Partenskii, M.B., M. Cai and P.C. Jordan, A dipolar chain model for the electrostatics of transmembrane ion channels 153 (1991) 125
Partenskii, M.B., M. Cai and P.C. Jordan, A dipolar chain model for the electrostatics of transmembrane ion channels, Chem. Phys. 153 (1991) 125–131. Erratum 154 (1991) 197
Partridge, H., see S.R. Langhoff 153 (1991) 1
Patron, F. and S.A. Adelman, Solvent cage effects and chemical dynamics in liquids 152 (1991) 121
Patsilinakou, E., D. Proch and C. Fotakis, Multiphoton dissociation dynamics of highly excited states of CS_2 and CS_2 clusters 153 (1991) 503
Pawlikowski, M. and O. Sonnich Mortensen, Symmetry and magnetic vibrational circular dichroism spectra of a doubly degenerate vibration and its combinations with non-degenerate vibrational modes 151 (1991) 73
Perchard, J.P., see H. Hannachi 154 (1991) 23
Perico, A., see Y. Hu 158 (1991) 395
Petelenz, P. and D. Mucha, Model calculations of the anthracene photocurrent spectrum 154 (1991) 145
Petelenz, P. and A. Eilmes, A cluster model of the charge transfer interaction between an impurity and the host molecular crystal 155 (1991) 247
Petelenz, P. and M. Slawik, Two-dimensional model of charge transfer excitons in polyacene crystals 157 (1991) 169
Petrovic, Z.Lj., see S.B. Vrhovac 153 (1991) 233
Pettersson, L.G.M., see H. Åkeby 155 (1991) 197
Peyerimhoff, S.D., see A. Banichevich 154 (1991) 199
Peyerimhoff, S.D., see W. Reuter 160 (1992) 11
Pfanstiel, J.F., see B.B. Champagne 156 (1991) 251
Philipp, R., see R.D. Young 158 (1991) 315
Pierre, M., P.L. Baldeck, D. Block, R. Georges, H.P. Trommsdorff and J. Zyss, Electronic spectra of 4-nitro-pyridine-*n*-oxide (NPO) single crystals 156 (1991) 103
Pine, A.S., see G.T. Fraser 156 (1991) 523
Pintar, M.M., see W.T. Sobol 152 (1991) 337
Pique, J.P., see M. Lombardi 156 (1991) 163
Plata, J., see E. Alvira 155 (1991) 7
Plaza, P., see M.M. Martin 153 (1991) 297
Pliva, J., see E. Riedle 152 (1991) 375

Plombon, J., see R.H. Austin 158 (1991) 473
Plusquellic, D.F., see B.B. Champagne 156 (1991) 251
Podgornik, R. and V.A. Parsegian, An electrostatic-surface stability interpretation of the "hydrophobic" force inferred to occur between mica plates in solutions of soluble surfactants 154 (1991) 477
Polák, R., An extended diatomics-in-molecules model for NH_2^+ 153 (1991) 91
Polinger, V.Z., N.N. Gorinchoi and I.B. Bersuker, MO LCAO analysis of the vibronic instability of the $CuCl_5^{3-}$ trigonal bipyramidal configuration. Critical view on the angular overlap model in vibronic problems 159 (1992) 75
Pongpituk, V., see K.P. Sagarik 156 (1991) 439
Ponterini, G. and F. Momicchioli, Trans–cis photoisomerization mechanism of carbocyanines: experimental check of theoretical models 151 (1991) 111
Ponterini, G., see I. Baraldi 160 (1992) 85
Popielawski, J., see A.S. Cukrowski 159 (1992) 39
Port, H., see K. Ulrich 154 (1991) 311
Pratt, D.W., see B.B. Champagne 156 (1991) 251
Pravilov, A.M., see A.B. Alekseyev 155 (1991) 173
Prencipe, M., see R. Dovesi 156 (1991) 11
Procacci, P., see A. Tafi 151 (1991) 205
Procacci, P., A. Tafi, L. Angeloni, R. Righini and P.R. Salvi, Vibrational relaxation in crystal SO_2 154 (1991) 331
Proch, D., see E. Patsilinakou 153 (1991) 503
Puccetti, G., I. Ledoux, J. Zyss, A. Jutand and C. Amatore, Measurement of quadratic hyperpolarizabilities of unsymmetrical donor–acceptor bi- and polyaryls: effect of size and torsion angle of aryl units 160 (1992) 467
Purtov, P.A., see A.B. Doktorov 160 (1992) 223
Purtov, P.A., see A.B. Doktorov 160 (1992) 239
Pusztai, L., see G. Tóth 160 (1992) 405

Rabitz, H., see J.P. Leroy 154 (1991) 395
Radovanov, S.B., see S.B. Vrhovac 153 (1991) 233
Raineri, F.O., Y. Zhou, H.L. Friedman and G. Stell, Ion solvation dynamics in an interaction-site model solvent 152 (1991) 201
Ramondo, F., L. Bencivenni, R. Caminiti and C. Sadun, Ab initio SCF study on $LiClO_4$ and Li_2SO_4 molecules: geometries and vibrational frequencies 151 (1991) 179
Ramondo, F., L. Bencivenni and V. Di Martino, Ab initio study on the coordination structures of $M^+XY_3^-$ and $M^+XY_4^-$ ion pairs 158 (1991) 41
Rao, C.N.R., see S. Yashonath 155 (1991) 351
Ratajczak, H., see J. Moc 159 (1992) 197
Rayez, J.C., see M. Monnerville 159 (1992) 227
Raynaud, M., C. Reynaud, Y. Ellinger, G. Hennico and J. Delhalle, Acrylonitrile versus allyl cyanide: the role of electronic conjugation in high electric field condition 153 (1991) 39
Recker, K., see D. Reinen 155 (1991) 117
Reinen, D., G. Steffen, M.A. Hitchman, H. Stratemeier, L. Dubicki, E.R. Krausz, M.J. Riley, H.E. Mathies, K. Recker and F. Wallrafen, The optical spectrum of $Ba_2Zn[Cu]F_6$ 155 (1991) 117
Reinen, D. and M. Atanasov, Symmetry and vibronic coupling: the stereochemistry and the ground state potential surface of Cu^{2+} in five-coordination 155 (1991) 157
Remacle, F., M. Desouter-Lecomte and J.C. Lorquet, Quantum effects in competitive unimolecular reactions 153 (1991) 201
Rettschnick, R.P.H., see G.-J. Kroes 156 (1991) 293
Reuss, J., see R. Engeln 156 (1991) 215
Reuss, J., see R. Engeln 160 (1992) 427
Reuter, W. and S.D. Peyerimhoff, Ab initio study of the vibrational structure of the X^2A_1 and A^2B_1 electronic states of CH_2^+ 160 (1992) 11
Rey, A. and J. Skolnick, Comparison of lattice Monte Carlo dynamics and Brownian dynamics folding pathways of α-helical hairpins 158 (1991) 199
Rey, R., see E. Guàrdia 155 (1991) 187
Reynaud, C., see M. Raynaud 153 (1991) 39
Richter, H., see H. Knöckel 152 (1991) 399
Richter, H., H. Knöckel and E. Tiemann, The potential of the Na_2 $B\,^1\Pi_u$ state 157 (1991) 217
Ridley, T., see P.J. Jewsbury 151 (1991) 103
Riedl, W., see R. Treichler 153 (1991) 259
Riedle, E. and J. Pliva, Mixing of the vibrational angular momentum components of multiply degenerate vibronic states of benzene by vibrational *l*-type resonance 152 (1991) 375
Riggi, F., see R.P. Bonomo 151 (1991) 323
Righetti, M.C., see L.B. Favero 155 (1991) 107
Righini, R., see G.F. Signorini 154 (1991) 245
Righini, R., see P. Procacci 154 (1991) 331
Riley, M.J., see D. Reinen 155 (1991) 117
Robert, D., see S. Temkin 158 (1991) 89
Robinson, G.W., see S.-B. Zhu 152 (1991) 221
Rode, B.M., see Y.P. Yongyai 156 (1991) 403
Roetti, C., see R. Dovesi 156 (1991) 11
Rom, N., N. Lipkin and N. Moiseyev, Optical potentials by the complex coordinate method 151 (1991) 199
Rościszewski, K., M. Chaumet and P. Fulde, Estimation of electronic correlation energies and binding energies for molecules composed of first-row atoms 151 (1991) 159

Rosi, M., C.W. Bauschlicher Jr. and S.R. Langhoff, Theoretical study of the spectroscopy of Al_2^+ 151 (1991) 1
Rosmus, P., see I. Fischer 151 (1991) 295
Rosmus, P., see Th. Glenewinkel-Meyer 152 (1991) 409
Roszak, S. and J.J. Kaufman, Ab-initio multiple reference double-excitation configuration-interaction ground and excited state potential curves for the $H_2N–NO_2$ decomposition in nitramine 160 (1992) 1
Rothamel, F., see B. Stein 159 (1992) 269
Rudziński, J.M., see J. Moc 159 (1992) 197
Rühl, E. and A.P. Hitchcock, Oxygen K-shell excitation spectroscopy of hydrogen peroxide 154 (1991) 323
Rühl, E., see R. Locht 160 (1992) 477
Ruiz-López, M.F., see F. Bohr 156 (1991) 55
Rusiloski, B.E., see D.B. Chesnut 157 (1991) 105

Sadeghi, N., see P. Kowalczyk 160 (1992) 73
Sadlej, A.J., see V. Kellö 157 (1991) 123
Sadlej, A.J., see G.H.F. Diercksen 158 (1991) 9
Sadlej, A.J., see G.H.F. Diercksen 158 (1991) 19
Sadun, C., see F. Ramondo 151 (1991) 179
Sagarik, K.P., V. Pongpituk, S. Chaiyapongs and P. Sisot, Test-particle model potentials for hydrogen-bonded complexes: complexes formed from HCN, HF, H_2O, NH_3, $HCONH_2$, $HCONHCH_3$, guanine and cytosine 156 (1991) 439
Saint-Espès, C., X. Chapuisat and F. Schneider, A weak-mode representation of floppy molecules. I. Potential energy 159 (1992) 377
Saint-Espès, C., see X. Chapuisat 159 (1992) 391
Saito, G., see T. Ida 156 (1991) 113
Saito, G., see T. Ida 157 (1991) 305
Salaneck, W.R., see N. Sato 160 (1992) 299
Salvi, P.R., see A. Tafi 151 (1991) 205
Salvi, P.R., see P. Procacci 154 (1991) 331
Samios, J., H. Stassen and T. Dorfmüller, Test of effective pair potential models by molecular dynamics simulation on liquid OCS 160 (1992) 33
Sandker, G.J., see J.P.J. Driessen 155 (1991) 447
San Fabián, E., see J.M. García de la Vega 151 (1991) 335
Sanna, N., see F.A. Gianturco 158 (1991) 77
Sato, N. and M. Yoshikawa, UV photoemission spectroscopic studies on molecular aggregation of triphenylamines dispersed in polycarbonate thin films 160 (1992) 289
Sato, N., M. Lögdlund, R. Lazzaroni, W.R. Salaneck, J.-L. Brédas, D.D.C. Bradley, R.H. Friend and K.E. Ziemelis, The electronic structure of poly(*p*-phenylene vinylene) 160 (1992) 299
Sato, T., see G. Biesmans 160 (1992) 97
Sauer, S.P.A., V. Špirko and J. Oddershede, The magnetizability and *g*-factor surfaces of ammonia 153 (1991) 189
Saunders, V.R., see R. Dovesi 156 (1991) 11
Šavrda, J., see J. Vojtík 156 (1991) 369
Schaefer III, H.F., see M. Shen 151 (1991) 187
Schanne, P., see G.M. Gale 151 (1991) 127
Schanne, P. and G.M. Gale, Interference and Fermi-resonant two-vibron bound states 159 (1992) 1
Schettino, V., see G.F. Signorini 154 (1991) 245
Schlachta, R., G. Lask, S.H. Tsay and V.E. Bondybey, Pulsed discharge source of supersonically cooled transient species 155 (1991) 267
Schleipen, J. and J.J. ter Meulen, State-to-state cross sections for rotational excitation of ortho- and para-NH_3 by He and H_2 156 (1991) 479
Schlyer, B.D., see M. Yagi 157 (1991) 209
Schmid, D., see A. Krüger 157 (1991) 243
Schmidt, R., see A.S. Cukrowski 159 (1992) 39
Schneider, F., see C. Saint-Espès 159 (1992) 377
Schneider, W. and W. Thiel, Ab initio calculation of anharmonic force fields for the methyl, silyl, germyl, and stannyl halides 159 (1992) 49
Scholes, G.D., K.P. Ghiggino and G.J. Wilson, Excimer geometries in bichromophoric molecules: a theoretical and experimental study of 1,2-(bis-9-antrhyl)-ethane 155 (1991) 127
Scholl, R., see R.D. Young 158 (1991) 315

Schroeder, J., see Ch. Gehrke 152 (1991) 45
Schüle, J., see M. Ohno 158 (1991) 1
Schulten, K. and M. Tesch, Coupling of protein motion to electron transfer: molecular dynamics and stochastic quantum mechanics study of photosynthetic reaction centers 158 (1991) 421
Schulze, K.D., Simulation of the unstable dynamics of excitable biomembranes: properties of a cyclic electrochemical gating mechanism 156 (1991) 43
Schurath, U., see M. Winter 159 (1992) 235
Schurath, U., see K. Seranski 159 (1992) 247
Schurr, J.M., see L. Song 155 (1991) 63
Schweig, A., see K. Kesper 153 (1991) 511
Schweig, A., see J. Kreile 155 (1991) 99
Scully, A.D., A. Matsumoto and S. Hirayama, A time-resolved fluorescence study of electronic excitation energy transport in concentrated dye solutions 157 (1991) 253
Scully, A.D., H. Yasuda, M. Okamoto and S. Hirayama, The effect of pressure on the dynamic quenching by oxygen of the excited singlet state of 9,10-dimethylanthracene in solution 157 (1991) 271
Searles, D., see R. Eggenberger 156 (1991) 395
Sears, T.J., see U. Bley 152 (1991) 281
Seel, M. and W. Domcke, Model studies on femtosecond time-resolved ionization spectroscopy of excited-state vibrational dynamics and vibronic coupling 151 (1991) 59
Seibel, W., see J. Kreile 155 (1991) 99
Seibt, W., see Y. Luo 153 (1991) 473
Seidl, M., J. Kaa and M. Maier, Relaxation of singlet molecular oxygen in the liquid and gas phase up to 154 K 157 (1991) 279
Seliger, J., see E. Hadjoudis 156 (1991) 149
Semmes, D.H., see A. Heikal 156 (1991) 231
Seranski, K., see M. Winter 159 (1992) 235
Seranski, K., M. Winter and U. Schurath, Site-resolved vibronic spectra of matrix-isolated NBr: comparison with model calculations 159 (1992) 247
Serbutoviez, C., see M. Barzoukas 153 (1991) 457
Serna, I., see I. Urrecha 154 (1991) 85
Servens, C., see J.Y. Moisan 153 (1991) 465
Shafizadeh, N., see S. Guizard 156 (1991) 509
Shalabi, A.S., Nodal configurations and many-body energies in Li_3^{3+}, F_3^{3-}, $Li_2^{2+}F^-$ and $Li^+F_2^{2-}$ ions at crystal and cluster geometries 156 (1991) 359
Shalev, E., see D. Bahatt 156 (1991) 223
Shen, J. and J.A. McCammon, Molecular dynamics simulation of superoxide interacting with superoxide dismutase 158 (1991) 191
Shen, M., Y. Xie, H.F. Schaefer III and C.A. Deakyne, The H_2O_2–NO_2^- and $H_2NO_4^-$ isomers of the nitrate anion–water complex 151 (1991) 187
Shestakov, O.D., see A.B. Alekseyev 155 (1991) 173
Shin, K.J., see S. Lee 156 (1991) 339
Shkrob, I.A., V.F. Tarasov and E.G. Bagryanskaya, Electron spin exchange in micellized radical pairs. I. ^{13}C low field chemically induced dynamic nuclear polarization (CIDNP) and ^{13}C radio frequency stimulated nuclear polarization (SNP) 153 (1991) 427
Shkrob, I.A., V.F. Tarasov and A.L. Buchachenko, Electron spin exchange in micellized radical pairs. II. Magnetic field and magnetic isotope effects in multinuclear pairs 153 (1991) 443

Shlihta, G.A., see E.A. Silinsh 155 (1991) 389
Shokhirev, N.V., E.C. Korolenko, M.B. Taraban and T.V. Leshina, Anomalous magnetic effects. The role of association in the recombination of singlet radical pairs in liquids 154 (1991) 237
Shreve, A.P., J.K. Trautman, T.G. Owens and A.C. Albrecht, A femtosecond study of electronic state dynamics of fucoxanthin and implications for photosynthetic carotenoid-to-chlorophyll energy transfer mechanisms 154 (1991) 171
Shushin, A.I., Net CIDNP in geminate radical pair recombination in viscous liquids. Comparison of theory and experiment for high magnetic fields 152 (1991) 133
Siegbahn, K., see Y. Luo 153 (1991) 473
Siegbahn, P., see O. Swang 156 (1991) 379
Signorini, G.F., R. Righini and V. Schettino, Lattice dynamics of the orthorhombic phase of $KClO_4$: Ewald's method in molecular coordinates 154 (1991) 245
Silinsh, E.A., G.A. Shlihta and A.J. Jurgis, A model description of charge carrier transport phenomena in organic molecular crystals. II. Perylene 155 (1991) 389
Silvi, B., see H. Hannachi 154 (1991) 23
Simas, A.M., see H.F.M. da Costa 154 (1991) 379
Simon, J.D. and S.-G. Su, Picosecond Stokes shift studies of solvent friction: experimental measurements of time-dependent band shape and integrated intensity 152 (1991) 143
Simon, J.G.G., see K. Kesper 153 (1991) 511
Simpson, C.J.S.M., see J.J. Andrew 153 (1991) 247
Singh, S., see S.-B. Zhu 152 (1991) 221
Sisot, P., see K.P. Sagarik 156 (1991) 439
Sjöqvist, L., N.P. Benetis, A. Lund and J. Maruani, Intramolecular dynamics of the C_4H_8NH radical cation. An application of the anisotropic exchange theory for powder ESR lineshapes 156 (1991) 457
Skolnick, J., see A. Rey 158 (1991) 199
Slaman, M.J. and R.A. Aziz, Quantum effects on thermal diffusion factors at room temperature for some noble gas pairs 154 (1991) 33
Slawik, M., see P. Petelenz 157 (1991) 169
Sloan, J.J., see P.J. Kuntz 151 (1991) 77
Smedarchina, Z., see L. Lavtchieva 160 (1992) 211
Smith, P.W., see R.G. McDonald 154 (1991) 179
Snider, N., Energy transfer distributions for classical, collinear atom–diatom collisions 159 (1992) 339
Sobol, W.T., I.G. Cameron and M.M. Pintar, A Zeeman level crossing study of the symmetry of the potential hindering the torsional oscillator CH_3 152 (1991) 337
Sobolewski, A.L., see A. Staib 156 (1991) 21
Softley, T.P., see H.H. Fielding 155 (1991) 257
Someya, K., see K. Tanaka 152 (1991) 229
Song, L. and J.M. Schurr, Three-time autocorrelation function of the power associated with a Gaussian random process 155 (1991) 63
Sonnich Mortensen, O., see M. Pawlikowski 151 (1991) 73
Soto, M.R., M. Page and M.L. McKee, Theoretical study of the reaction of OH with HNO 153 (1991) 415
Spalletti, A., G. Bartocci, F. Masetti, U. Mazzucato and G. Cruciani, Principal-component self-modeling analysis of fluorescence for some trans-diarylethylenes. A comparison with kinetic analysis 160 (1992) 131
Specht, H., see K. Kesper 153 (1991) 511
Speyer, J., see M.G. Usha 158 (1991) 487

Špirko, V., A. Čejchan and G.H.F. Diercksen, Rotation–vibration energies of FHF^- and $ClHCl^-$ from high-level correlated calculations of potential energy surfaces 151 (1991) 45
Špirko, V., see S.P.A. Sauer 153 (1991) 189
Staib, A., see M.C. Böhm 155 (1991) 27
Staib, A., W. Domcke and A.L. Sobolewski, Vibronic coupling in Rydberg series of linear molecules 156 (1991) 21
Stassen, H., see J. Samios 160 (1992) 33
Steffen, G., see D. Reinen 155 (1991) 117
Stein, B., F. Rothamel, T. Kirski, J. Kolenda and C. von Borczyskowski, Optical and ODMR spectroscopy of an induced triplet X-trap in 1,4-dibromobenzene single crystals 159 (1992) 269
Steinbach, P.J., R.J. Loncharich and B.R. Brooks, The effects of environment and hydration on protein dynamics: a simulation study of myoglobin 158 (1991) 383
Stekolnikov, A.V., see T.A. Cherepanova 154 (1991) 41
Stell, G., see Y. Zhou 152 (1991) 185
Stell, G., see F.O. Raineri 152 (1991) 201
Stephenson, J.C., see J.D. Beckerle 160 (1992) 487
Stiller, W., see A.S. Cukrowski 159 (1992) 39
Storozhev, A.V. and M.L. Strekalov, Relaxation cross sections for transfer of rotational angular momentum in a semiclassical approximation 153 (1991) 99
Stranger, R., see R.G. McDonald 154 (1991) 179
Stratemeier, H., see D. Reinen 155 (1991) 117
Straub, J.E. and M. Karplus, Molecular dynamics study of the photodissocation of carbon monoxide from myoglobin: ligand dynamics in the first 10 ps 158 (1991) 221
Strekalov, M.L., see A.V. Storozhev 153 (1991) 99
Su, M.-C., H.-K. O and C.S. Parmenter, A fluorescence characterization of the *p*-difluorobenzene–argon van der Waals complex. Energy levels, geometries and dissociation energies 156 (1991) 261
Su, S.-G., see J.D. Simon 152 (1991) 143
Suenram, R.D., see G.T. Fraser 156 (1991) 523
Sumpter, B.G. and D.W. Noid, Computational experiments on the intramolecular energy flow in macromolecules 160 (1992) 393
Sushkov, D.G., see V.V. Korolev 158 (1991) 129
Suter, H.U. and T.K. Ha, A theoretical study on the internal rotation and hyperfine structures of the ethyl radical (CH_3–CH_2) 154 (1991) 227
Suzuki, T., see A. Tachibana 156 (1991) 79
Svensson, S., see M.P. Keane 155 (1991) 379
Swang, O., K. Faegri Jr., O. Gropen, U. Wahlgren and P. Siegbahn, A theoretical study of the chemisorption of methane on a Ni(100) surface 156 (1991) 379

Tachibana, A., T. Suzuki, N. Yoshida, Y. Teramoto and T. Yamabe, New mechanism for the vibrational mode-specific proton-transfer reaction $NH_3^+(v)+NH_3 \rightarrow NH_2+NH_4^+$ 156 (1991) 79
Tafi, A., P. Procacci, E. Castellucci and P.R. Salvi, Polar phonons in SO_2 single crystal 151 (1991) 205
Tafi, A., see P. Procacci 154 (1991) 331
Tague Jr., T.J. and C.A. Wight, Laser-initiated chain reactions and microexplosions in solid solutions of methylcyclopropane and chlorine 156 (1991) 141
Tague Jr., T.J. and C.A. Wright, Laser-initiated chain reactions and microexplosions in solid solutions of methylcyclopropane and chlorine, Chem. Phys. 156 (1991) 141–148. Erratum 157 (1991) 305
Tan, K.H., see J.D. Bozek 158 (1991) 171
Tanaka, K., see Y. Mochizuki 151 (1991) 11
Tanaka, K., K. Someya and T. Tanaka, Observation of level crossing and level anticrossing signals in the CO_2 laser Stark spectrum of POF_3 and their proposed application to electric field standards in laser Stark spectroscopy 152 (1991) 229
Tanaka, T., see K. Tanaka 152 (1991) 229
Tang, K.T. and J.P. Toennies, A combining rule calculation of the van der Waals potentials of the rare-gas hydrides 156 (1991) 413
Tao, Y., Isomerization and unimolecular rearrangement channels of dithioformic acid 154 (1991) 221
Taraban, M.B., see N.V. Shokhirev 154 (1991) 237
Tarasov, V.F., see I.A. Shkrob 153 (1991) 427
Tarasov, V.F., see I.A. Shkrob 153 (1991) 443
Tarjus, G. and D. Kivelson, Solvent effect on activated rate processes: on the validity of the GLE approach 152 (1991) 153
Taylor, J.W., see F.A. Grimm 154 (1991) 303
Taylor, R., see S. Leach 160 (1992) 451
Tchougreeff, A.L. and I.A. Misurkin, Ferromagnetism of charge-transfer crystals 153 (1991) 371
Temkin, S., J.M. Thuet, L. Bonamy, J. Bonamy and D. Robert, Angular momentum and rotational energy relaxation in N_2–N_2 collisions calculated from coherent and stimulated Raman spectroscopy data 158 (1991) 89
Temme, F.P., see J.P. Colpa 154 (1991) 97
Temme, F.P. and J.P. Colpa, Structure of MQ-NMR spin spaces under higher $\mathscr{S}_n$- and $(\mathscr{S}_n)\downarrow\mathscr{G}$ symmetries. III. $\Gamma/\tilde{\Gamma}$ $((\mathscr{S}_7)\downarrow D_5)$ subduced irreps for $[A]_7$ clusters pertaining to the molecular cage ion, $[BH]_7^{2-}$ 154 (1991) 111
Temme, F.P., see J.P. Colpa 156 (1991) 532
Temps, F., see U. Bley 152 (1991) 281
Teramoto, Y., see A. Tachibana 156 (1991) 79
Ter Meulen, J.J., see J. Schleipen 156 (1991) 479
Tesch, M., see K. Schulten 158 (1991) 421
Thambir, C., see A.G. Adam 152 (1991) 391
Thiel, W., see D. Bakowies 151 (1991) 309
Thiel, W., see C. Kaupert 156 (1991) 85
Thiel, W., see W. Schneider 159 (1992) 49
Thorne, J.R.G., S.A. Williams, R.M. Hochstrasser and P.J. Fagan, Radiative lifetimes of confined excitations in sigma-conjugated silane oligomers 157 (1991) 401
Thuet, J.M., see S. Temkin 158 (1991) 89
Tiemann, E., see H. Knöckel 152 (1991) 399
Tiemann, E., see H. Richter 157 (1991) 217

Tiňo, J., see V. Klimo 159 (1992) 141
Toennies, J.P., see K.T. Tang 156 (1991) 413
Tokue, I., A. Masuda, H. Kume and Y. Ito, Rotational distributions of $N_2O^+(\tilde{A}^2\Sigma^+)$, $CO_2^+(\tilde{A}^2\Pi_u)$ and $CS_2^+(\tilde{A}^2\Pi_u)$ produced by electron-impact ionization 158 (1991) 161
Tomkinson, J., see F. Fillaux 154 (1991) 135
Tomkinson, J., see F. Fillaux 158 (1991) 113
Tondello, E., see M. Casarin 154 (1991) 385
Tondello, E., see M. Casarin 159 (1992) 365
Torchia, D.A., see H.B.R. Cole 158 (1991) 271
Tossell, J.A., Calculation of the inner shell excitation spectra and estimation of the electron scattering and dissociative attachment resonance energies of SF_6, SO_2, SF_2O, SF_2O_2, SF_4, SF_4O and S_2F_{10} 154 (1991) 211
Tóth, G. and L. Pusztai, Comparative studies of the underlying local order corresponding to different radial distribution functions of disordered materials 160 (1992) 405
Trajmar, S., see D.C. Cartwright 153 (1991) 219
Tramer, A., see C. Crépin 156 (1991) 281
Trautman, J.K., see A.P. Shreve 154 (1991) 171
Traytak, S.D., On the solution of the Debye–Smoluchowski equation with a Coulomb potential. III. The case of a Boltzmann initial distribution and a perfectly absorbing sink 154 (1991) 263
Treichler, R., W. Wurth, W. Riedl, P. Feulner and D. Menzel, Core excitation-induced photodesorption of molecular and fragment ions from CO adsorbates on metal surfaces 153 (1991) 259
Troe, J., see Ch. Gehrke 152 (1991) 45
Trommsdorff, H.P., see M. Pierre 156 (1991) 103
Tronc, M., see M. Ben Arfa 155 (1991) 143
Tronc, M., see C. Dezarnaud 156 (1991) 129
Trsic, M., see H.F.M. da Costa 154 (1991) 379
Tsay, S.H., see R. Schlachta 155 (1991) 267
Tsuboi, T., see T. Ogawa 156 (1991) 465
Tsuchiya, S., see N. Ochi 152 (1991) 319
Tsukada, M., see T. Ogawa 156 (1991) 473
Tsurubuchi, S., K. Motohashi, S. Matsuoka and T. Arikawa, Dissociative excitation of SiH_4 by electron impact: emission cross sections for the hydrogen Lyman series 155 (1991) 401
Turq, P., see J.L.F. Abascal 153 (1991) 79

Uijt de Haag, P., W.L. Meerts and J.T. Hougen, A study of the S_1 6^1 ($^1A_2''$) vibronically excited state of sym-triazine by high-resolution UV laser spectroscopy 151 (1991) 371
Uijt de Haag, P. and W.L. Meerts, Vibrational and rotational effects on the intersystem crossing in pyrazine and pyrimidine 156 (1991) 197
Ulrich, K., H. Port, H.C. Wolf, J. Wonner, F. Effenberger and H.-D. Ilge, Photochromic thiophenefulgides. Photokinetics of two isopropyl derivatives 154 (1991) 311
Ulstrup, J., see A.M. Kuznetsov 157 (1991) 25
Ulyanenkov, A.P., see I.D. Feranchuk 157 (1991) 61
Umemoto, H., see A. Masaki 158 (1991) 155
Urban, J., see V. Klimo 159 (1992) 141
Urban, M., see G.H.F. Diercksen 158 (1991) 19
Urrecha, I., I. Serna and J. Iturbe, Quasiclassical trajectory study of the two channels of the F+ICl system: effect of the collisional energy 154 (1991) 85
Usha, M.G., J. Speyer and R.J. Wittebort, Dynamics of the hydrate and amide groups of crystalline ribonuclease and lysozyme 158 (1991) 487
Uzhinov, B.M., see S.I. Druzhinin 158 (1991) 137

Valkunas, L., see A. Krüger 157 (1991) 243
Vančura, J. and Z. Herman, Hydroxonium ion formation in collisions of $H_2O^+ + D_2O$ and $D_2O^+ + H_2O$: a crossed-beam scattering study 151 (1991) 249
Van der Auweraer, M., see G. Biesmans 160 (1992) 97
Van der Zande, W.J., The vibrational constant of the $O_2^{2+} X\,^1\Sigma_g^+$ state from the dissociative decay of $n=3,4$ Rydberg states in O_2^+ 157 (1991) 287
Van der Zande, W.J., see J.H.M. Beijersbergen 160 (1992) 151
Van der Zwan, G. and J.T. Hynes, Chemical reaction rates and solvation dynamics in electrolyte solutions: ion atmosphere friction 152 (1991) 169
Van de Weijer, F.J.M., see J.P.J. Driessen 155 (1991) 447
Van Hemert, M.C., see A. Banichevich 154 (1991) 199
Van Herpen, W.M., see B.B. Champagne 156 (1991) 251
Van Oort, E. and M. Glasbeek, Fluorescence detected level-anticrossing and spin coherence of a localized triplet state in diamond 152 (1991) 365
Vasil'ev, O.V., see V.D. Lakhno 153 (1991) 147
Veenstra, B.R., H.C. Meijers, P.J. de Lange and J. Kommandeur, The structure of mixed watery clusters 156 (1991) 157
Verhaar, B.J., see J.P.J. Driessen 155 (1991) 447
Vervloet, M., see S. Leach 160 (1992) 451
Vilesov, A.F., J. Wildt and E.H. Fink, Emission of Xe:N(^{2}P) collision complexes near the N(^{2}P$\rightarrow\,^2$D) lines 153 (1991) 531
Vilesov, A.F., see J. Wildt 159 (1992) 127
Vinogradov, G.A., V.N. Likhachev and A.A. Ovchinnikov, Motion and geminal recombination of charged carriers in highly anisotropic three-dimensional systems (Onsager theory) 154 (1991) 367
Visticot, J.P., see J.M. Mestdagh 155 (1991) 79
Vittadini, A., see M. Casarin 154 (1991) 385
Vittadini, A., see M. Casarin 159 (1992) 365
Vöhringer, P., see Ch. Gehrke 152 (1991) 45
Vojtík, J., L. Češpiva, I. Paidarová and J. Šavrda, Nuclear quadrupole coupling constants of rovibrational levels of all isotopic species of BH^+ in their $X\,^2\Sigma^+$ and $B'\,^2\Sigma^+$ states 156 (1991) 369
Vojtík, J. and I. Paidarová, Modified version of the trajectory surface leaking method for dynamical calculations on autoionizing atom–diatom collision systems 157 (1991) 67
Von Borczyskowski, C., see B. Stein 159 (1992) 269
Von Niessen, W., see A.I. Boldyrev 155 (1991) 71
Von Niessen, W., see J. Mai 156 (1991) 63
Von Niessen, W., see M. Ohno 158 (1991) 1
Von Niessen, W., see W. Wardermann 159 (1992) 11
Vrhovac, S.B., S.B. Radovanov, S.A. Bzenić, Z.Lj. Petrović and B.M. Jelenković, Dissociative excitation of hydrogen in rf and dc glow discharges through H_2 153 (1991) 233

Wada, Y., see A. Masaki 158 (1991) 155
Wahlgren, U., see O. Swang 156 (1991) 379
Waits, L.D., R.J. Horwitz and J.A. Guest, Translational energy study of CH_3 photofragments following $^1(n,\pi^*)$ excitation of acetone 155 (1991) 149
Walker, G.C., see W. Jarzeba 152 (1991) 57
Walker, I.C. and M.H. Palmer, The electronic states of the azines. IV. Pyrazine, studied by VUV absorption, near-threshold electron energy-loss spectroscopy and ab initio multi-reference configuration interaction calculations 153 (1991) 169
Walker, I.C., see M.H. Palmer 157 (1991) 187
Walker, Z.H. and E.A. Ogryzlo, Kinetics of the reactions of intrinsic and phosphorus doped polycrystalline silicon with molecular chlorine 153 (1991) 483
Wallace, R., see J.P. Leroy 154 (1991) 395
Wallin, E. and L. Holmlid, Excited states of hydrogen emitted from a graphite diffusion source: Arrhenius behaviour 159 (1992) 313
Wallrafen, F., see D. Reinen 155 (1991) 117
Walton, D.R.M., see S. Leach 160 (1992) 451
Wang, N.S., see D.L. Yang 160 (1992) 307
Wang, N.S., see D.L. Yang 160 (1992) 317
Wang, Y., see G.H. Dai 155 (1991) 275
Wardermann, W. and W. von Niessen, Satellite lines at the ionization threshold in charge transfer systems 159 (1992) 11
Warshel, A., Z.T. Chu and J.-K. Hwang, The dynamics of the primary event in rhodopsins revisited 158 (1991) 303
Wayne, R.P., see J. Wildt 156 (1991) 497
Wayne, R.P., see J. Wildt 159 (1992) 127
Weaver, M.J., see G.E. McManis 152 (1991) 107
Werner, H.-J., see I. Fischer 151 (1991) 295
Werner, H.-J., see Th. Glenewinkel-Meyer 152 (1991) 409
Whalen, J.M., see H. Furue 154 (1991) 425
Whitley, T.A., see F.A. Grimm 154 (1991) 303
Wight, C.A., see T.J. Tague Jr. 156 (1991) 141
Wildt, J., see A.F. Vilesov 153 (1991) 531
Wildt, J., G. Bednarek, E.H. Fink and R.P. Wayne, Laser excitation of the $A^3\Sigma_u^+$, $A'^3\Delta_u$ and $c^1\Sigma_u^-$ states of molecular oxygen 156 (1991) 497
Wildt, J., E.H. Fink, P. Biggs, R.P. Wayne and A.F. Vilesov, Collision-induced emission of $O_2(a^1\Delta_g \rightarrow X^3\Sigma_g^-)$ in the gas phase 159 (1992) 127
Williams, I.H., see J.S. Francisco 160 (1992) 255
Williams, S.A., see J.R.G. Thorne 157 (1991) 401
Willmott, P.R., H. Bitto and J.R. Huber, Energy and rotational state dependence of radiationless processes in propynal 156 (1991) 177
Wilson, G.J., see G.D. Scholes 155 (1991) 127
Wilson, K.R., see I. Benjamin 152 (1991) 1
Winter, M., K. Seranski and U. Schurath, Site effects in spectra of matrix-isolated diatomic molecules: a modelling approach 159 (1992) 235
Winter, M., see K. Seranski 159 (1992) 247
Wittebort, R.J., see M.G. Usha 158 (1991) 487
Wittneben, V., see P. Mottner 160 (1992) 327

Wolf, H.C., see K. Ulrich 154 (1991) 311
Wolynes, P.G., see C. Zheng 158 (1991) 261
Wonner, J., see K. Ulrich 154 (1991) 311
Woodward, C.E. and B. Jönsson, Monte Carlo and mean field studies of a polyelectrolyte in salt solution 155 (1991) 207
Wormell, P. and A.R. Lacey, Electronic spectra of the naphthyridines: 2,7-naphthyridine 160 (1992) 55
Wright, C.A., see T.J. Tague Jr. 157 (1991) 305
Wright, J.S., see P.J. Bruna 157 (1991) 111
Wurth, W., see R. Treichler 153 (1991) 259

Xie, Y., see M. Shen 151 (1991) 187
Xing, K.Z., see Y. Luo 153 (1991) 473

Yagi, M., B.D. Schlyer and A.H. Maki, Optically detected magnetic resonance study of the phosphorescent states of trans-2,2′-bipyridine, metal-free cis-2,2′-bipyridine and $[Zn(bpy)]^{2+}$ 157 (1991) 209
Yakushi, K., see T. Ida 156 (1991) 113
Yakushi, K., see T. Ida 157 (1991) 305
Yamabe, T., see A. Tachibana 156 (1991) 79
Yamochi, H., see T. Ida 156 (1991) 113
Yamochi, H., see T. Ida 157 (1991) 305
Yan, Q.J., see G.H. Dai 155 (1991) 275
Yáñez, M., see M. Alcamí 151 (1991) 21
Yang, D.L., T. Yu, N.S. Wang and M.C. Lin, Temperature dependence of cyanogen radical reactions with selected alkanes: CN reactivities towards primary, secondary and tertiary C–H bonds 160 (1992) 307
Yang, D.L., T. Yu, N.S. Wang and M.C. Lin, CN radical reactions with selected olefins in the temperature range 174–740 K 160 (1992) 317
Yang, M., see S. Lee 156 (1991) 339
Yang, M., see A.M. Ahmed 158 (1991) 329
Yashonath, S. and C.N.R. Rao, Structure and dynamics of polar liquids: a molecular dynamics investigation of N,N-dimethyl formamide 155 (1991) 351
Yasuda, H., see A.D. Scully 157 (1991) 271
Ye, L., A.J. Freeman and B. Delley, Local density functional study of the structural and electronic properties of C_{60} and XC_{60} (X=K, Rb, Cs) 160 (1992) 415
Yi, X., see S. Lin 160 (1992) 163
Yonezawa, Y., see G. Biesmans 160 (1992) 97
Yongyai, Y.P., S. Kokpol and B.M. Rode, Zinc ion in water: intermolecular potential with approximate three-body correction and Monte Carlo simulation 156 (1991) 403
Yoshida, N., see A. Tachibana 156 (1991) 79
Yoshikawa, M., see N. Sato 160 (1992) 289
Young, R.D., H. Frauenfelder, J.B. Johnson, D.C. Lamb, G.U. Nienhaus, R. Philipp and R. Scholl, Time- and temperature dependence of large-scale conformational transitions in myoglobin 158 (1991) 315
Yu, T., see D.L. Yang 160 (1992) 307
Yu, T., see D.L. Yang 160 (1992) 317

Zachilas, L. and S.C. Farantos, Periodic orbits and quantum localization in the van der Waals systems CO–Ar 154 (1991) 55
Zagar, V., see E. Hadjoudis 156 (1991) 149
Zewail, A.H., see A. Heikal 156 (1991) 231
Zhang, W., G. Cooper, T. Ibuki and C.E. Brion, Excitation and ionization of freon molecules. II. Absolute oscillator strengths for the photoabsorption (7.5–200 eV) and the ionic photofragmentation (12.5–80 eV) of CF_3Cl 151 (1991) 343
Zhang, W., G. Cooper, T. Ibuki and C.E. Brion, Excitation and ionization of freon molecules. III. Absolute oscillator strengths for the photoabsorption (8.5–200 eV) and the ionic photofragmentation (11.5–70 eV) of CF_2Cl_2 151 (1991) 357
Zhang, W., G. Cooper, T. Ibuki and C.E. Brion, Excitation and ionization of freon molecules. IV. Absolute oscillator strengths for the photoabsorption (6–200 eV) and the ionic photofragmentation (11.5–49 eV) of $CFCl_3$ 153 (1991) 491
Zhang, W., T. Ibuki and C.E. Brion, Absolute dipole differential oscillator strengths for inner shell spectra from high resolution electron energy loss studies of the freon molecules CF_4, CF_3Cl, CF_2Cl_2, $CFCl_3$ and CCl_4 160 (1992) 435
Zharikov, A.A., see A.I. Burshtein 152 (1991) 23
Zharikov, A.A., see A.I. Burshtein 155 (1991) 91
Zheng, C., J.A. McCammon and P.G. Wolynes, Quantum simulation of conformation reorganization in the electron transfer reactions of tuna cytochrome c 158 (1991) 261
Zhou, Y., H.L. Friedman and G. Stell, Outer-sphere electron-transfer reactions in model molecular solvents: the mean spherical approximation 152 (1991) 185
Zhou, Y., see F.O. Raineri 152 (1991) 201
Zhu, H., see T. Daniels 159 (1992) 289
Zhu, S.-B., S. Singh, J. Lee and G.W. Robinson, Velocity dependence of friction 152 (1991) 221
Zhu, X.R. and J.M. Harris, Photothermal grating spectroscopy study of nongeminate atom recombination of photodissociated iodine in liquids 157 (1991) 409
Ziemelis, K.E., see N. Sato 160 (1992) 299
Zitserman, V.Yu., see A.M. Berezhkovskii 157 (1991) 141
Zwart, E. and W.L. Meerts, The submillimeter rotation-tunneling spectrum of Ar–D_2O and Ar–NH_3 151 (1991) 407
Zyss, J., see M. Pierre 156 (1991) 103
Zyss, J., see G. Puccetti 160 (1992) 467

Subject Index to Volumes 151–160

Methods

Theoretical

Group theory and algebras

Structure of MQ-NMR spin spaces under higher $\mathcal{S}_n$- and $(\mathcal{S}_n)_{\downarrow}\mathcal{G}$ symmetries. II. $\Gamma/\tilde{\Gamma}$ $(\mathcal{S}_6)_{\downarrow}\mathcal{O}$ subduced irreps for sixfold spin clusters pertaining to the molecular cage ion, $[^{11}BH]_6^{2-}$, J.P. Colpa and F.P. Temme 154 (1991) 97
Structure of MQ-NMR spin spaces under higher $\mathcal{S}_n$- and $(\mathcal{S}_n)_{\downarrow}\mathcal{G}$ symmetries. III. $\Gamma/\tilde{\Gamma}$ $((\mathcal{S}_7)_{\downarrow}D_5)$ subduced irreps for $[A]_7$ clusters pertaining to the molecular cage ion, $[^{11}BH]_7^{2-}$, F.P. Temme and J.P. Colpa 154 (1991) 111
Structure of MQ-NMR spin spaces under higher $\mathcal{S}_n$- and $(\mathcal{S}_n)_{\downarrow}\mathcal{G}$ symmetries. II. $\Gamma/\tilde{\Gamma}$ $(\mathcal{S}_6)_{\downarrow}\mathcal{O}$ subduced irreps for sixfold spin clusters pertaining to the molecular cage ion, $[^{11}BH]_6^{2-}$, Chem. Phys. 154 (1991) 97–110. Erratum, J.P. Colpa and F.P. Temme 156 (1991) 532
Theory and simulation of optically induced line shifts in NMR, M.W. Evans 157 (1991) 1
Lie algebraic approach to scattering of molecules from a solid surface, S. Lin, X. Yi and L. Cai 160 (1992) 163

Classical mechanics

A multisurface classical trajectory study of the dynamics of the reaction $O(^1D_2)+H_2\rightarrow OH(v', J', \Theta')+H$ using the diatomics in molecules method, P.J. Kuntz, B.I. Niefer and J.J. Sloan 151 (1991) 77
An exact theory of friction for reactive collisions in a solvent using an interaction representation, D.M. Charutz and R.D. Levine 152 (1991) 31
Trajectory capture rate coefficients for ion–quadrupolar molecule reactions, I. Mendaš and P. Milutinović 153 (1991) 73
Periodic orbits and quantum localization in the van der Waals systems CO–Ar, L. Zachilas and S.C. Farantos 154 (1991) 55
New mechanism for the vibrational mode-specific proton-transfer reaction $NH_3^+(v)+NH_3\rightarrow NH_2+NH_4^+$, A. Tachibana, T. Suzuki, N. Yoshida, Y. Teramoto and T. Yamabe 156 (1991) 79
Coupling of protein motion to electron transfer: molecular dynamics and stochastic quantum mechanics study of photosynthetic reaction centers, K. Schulten and M. Tesch 158 (1991) 421
The effects of solvent on the conformation and the collective motions of protein: normal mode analysis and molecular dynamics simulations of melittin in water and in vacuum, A. Kitao, F. Hirata and N. Gō 158 (1991) 447
Two-dimensional trajectories of tunneling in the symmetric double-well potential, V.A. Benderskii, V.I. Goldanskii and D.E. Makarov 159 (1992) 29
Quasiclassical trajectory study of the effect of reactant rotation on the reaction $B^+ + HD\rightarrow BH^+(BD^+)+D(H)$, V. Klimo, J. Urban and J. Tiňo 159 (1992) 141
The dynamics of dressed variables, D.M. Charutz and R.D. Levine 159 (1992) 321

The importance of periodic orbits in analysing photodissociation resonances: the O_3 case, S.C. Farantos 159 (1992) 329
Energy transfer distributions for classical, collinear atom–diatom collisions, N. Snider 159 (1992) 339

Quantized field theory
Electron transfer induced by liquid defect motion. Exact solution, D.V. Matyushov 155 (1991) 331

Many body and quasiparticle approaches
Estimation of electronic correlation energies and binding energies for molecules composed of first-row atoms, K. Rościszewski, M. Chaumet and P. Fulde 151 (1991) 159
Time-dependent fluorescence depolarization arising from exciton annihilation in confined molecular domains, G. Juzeliūnas 151 (1991) 169
Symmetry breaking in thermally activated NH_4 rotation studied by NMR level crossing spectroscopy, S. Clough, A.J. Horsewill, M.R. Johnson, M.A. Mohammed and T. Newton 152 (1991) 343
The solvated electron in an electrolyte solution, V.D. Lakhno and O.V. Vasil'ev 153 (1991) 147
Ferromagnetism of charge-transfer crystals, A.L. Tchougreeff and I.A. Misurkin 153 (1991) 371
Calculation of excitation energies using quasidegenerate variational perturbation theory and multireference-averaged coupled-pair functional theory, M.A. Anderson and R.J. Cave 154 (1991) 1
Analytical potential energy surface for methane in terms of interatomic forces, H. Furue, J.F. LeBlanc, P.D. Pacey and J.M. Whalen 154 (1991) 425
Material properties of low-dimensional charge-transfer salts. I. Charge fluctuations in systems with stronger electronic correlations, M.C. Böhm and A. Staib 155 (1991) 27
The first ionization potentials of some MH_{k+1}^- and $M_2H_{2k+1}^-$ anions calculated by a Green's function method, A.I. Boldyrev and W. von Niessen 155 (1991) 71
Hole pairing on oxygen sites in high-T_c copper–oxide superconductors induced by an effective exchange interaction: a theoretical and numerical investigation on planar lattices, A. Ferretti and A. Lami 155 (1991) 179
Many-body calculations of the core hole spectra of NiCO, M. Ohno and P. Decleva 156 (1991) 309
Nodal configurations and many-body energies in Li_3^{3+}, F_3^{3-}, $Li_2^{2+}F^-$ and $Li^+F_2^{2-}$ ions at crystal and cluster geometries, A.S. Shalabi 156 (1991) 359
Interaction potentials in rare gas–halide ion systems, V. Kellö and A.J. Sadlej 157 (1991) 123
Two-dimensional model of charge transfer excitons in polyacene crystals, P. Petelenz and M. Slawik 157 (1991) 169
The treatment of electron correlation in aperiodic systems. IV. Exciton bands and double ionization potentials, C.-M. Liegener 157 (1991) 183
Many-body calculation of the valence photoemission spectrum of ferrocene, M. Ohno, W. von Niessen and J. Schüle 158 (1991) 1
Interference and Fermi-resonant two-vibron bound states, P. Schanne and G.M. Gale 159 (1992) 1
Satellite lines at the ionization threshold in charge transfer systems, W. Wardermann and W. von Niessen 159 (1992) 11
Chemical potential, partial enthalpy and partial volume of mixtures by *NPT* molecular dynamics, D.M. Heyes 159 (1992) 149
The dynamics of dressed variables, D.M. Charutz and R.D. Levine 159 (1992) 321
The Pariser–Parr–Pople model for trans-polyenes. I. Ab initio and semiempirical study of the bond alternation in trans-butadiene, W. Förner 160 (1992) 173
Many-body calculation of the XPS core hole spectra of NiN_2, P. Decleva and M. Ohno 160 (1992) 341

Many-body calculation of the core hole spectra of PdCO, P. Decleva and M. Ohno 160 (1992) 353

Coupling schemes and perturbative treatments

The diagmagnetic properties of the $\cdot NF_2$ radical by magic doublet rotational Zeeman spectroscopy, U.E. Frank and W. Hüttner 152 (1991) 261

Electron relaxation dynamics of Mu ALCR spectra, S.R. Kreitzman 152 (1991) 353

On the Jahn–Teller coupling of an orbital triplet with a vibrational doublet, E. Ghelichkhani and E.R. Grant 153 (1991) 133

Relation between total energy and sum of orbital energies for neutral atoms, A. Nagy and N.H. March 153 (1991) 141

Doppler-free radio frequency lineshape theory for a three-level system with three allowed transitions in presence of an IR pump, S. Ghoshal and A. Datta 153 (1991) 161

Theory of multiquantum optically detected ESR spectra of radical pairs. I. General theory. Resonances in parallel radio-frequency field, V.A. Morozov and A.B. Doktorov 153 (1991) 313

Theory of multiquantum optically detected ESR spectra of radical pairs. II. Resonances in perpendicular radio-frequency field, V.A. Morozov and A.B. Doktorov 153 (1991) 333

Generalized Einstein relations for ions in molecular gases, A.D. Koutselos and E.A. Mason 153 (1991) 351

Energy levels of Cr^{3+} ions in C_{3i} sites of $Y_3Al_5O_{12}$, C.A. Morrison, J.B. Gruber and M.E. Hills 154 (1991) 437

Semiempirical electrostatic polarization model of the ionic bonding in alkali and alkaline earth hydroxides and halides, J.M. Mestdagh and J.P. Visticot 155 (1991) 79

Symmetry and vibronic coupling: the stereochemistry and the ground state potential surface of Cu^{2+} in five-coordination, D. Reinen and M. Atanasov 155 (1991) 157

Theoretical study of the $HeH(B^2\Pi)$ fluorescence and predissociation, A.B. Alekseyev, V.S. Ivanov, A.M. Pravilov and O.D. Shestakov 155 (1991) 173

Vibronic coupling in Rydberg series of linear molecules, A. Staib, W. Domcke and A.L. Sobolewski 156 (1991) 21

Scaling the WCA reference system for two-dimensional Lennard-Jones fluids, F. Cuadros and A. Mulero 156 (1991) 33

Theory and simulation of optically induced line shifts in NMR, M.W. Evans 157 (1991) 1

Dissipative relaxation of a low-energy intermediate electronic state in three-level electron transfer, A.M. Kuznetsov and J. Ulstrup 157 (1991) 25

Construction of bound-state potential energy curves of diatomic molecules from spectroscopic data, C.G. Diaz, F.M. Fernández and E.A. Castro 157 (1991) 35

Absorption spectra of a solvated electron in ethers, H. Abramczyk and J. Kroh 157 (1991) 373

Driven damped harmonic oscillators perturbed by the parity operator, P. Blaise, M. Giry and O. Henri-Rousseau 159 (1992) 169

Generalized golden rule approach to the H-transfer problem. II. Application to a photochemical reaction, L. Lavtchieva and Z. Smedarchina 160 (1992) 211

The formulae for calculation of *g*-tensor shifts in third-order perturbation theory, E.N. Heifets 160 (1992) 363

Relativistic quantum mechanics

Potential curves and predissociation rates for the heavy species HBr^{2+} and DBr^{2+}, A. Banichevich, S.D. Peyerimhoff, B.A. Hess and M.C. van Hemert 154 (1991) 199

Transport quantum mechanics
Symmetry breaking in thermally activated NH_4 rotation studied by NMR level crossing spectroscopy, S. Clough, A.J. Horsewill, M.R. Johnson, M.A. Mohammed and T. Newton 152 (1991) 343
Low-temperature chemical reactions. Effect of symmetrically coupled vibrations in collinear exchange reactions, V.A. Benderskii, V.I. Goldanskii and D.E. Makarov 154 (1991) 407
Spatial dispersion of electron transfer probability, A.I. Burshtein, P.A. Frantsuzov and A.A. Zharikov 155 (1991) 91
Two-dimensional trajectories of tunneling in the symmetric double-well potential, V.A. Benderskii, V.I. Goldanskii and D.E. Makarov 159 (1992) 29
Theory of geminate recombination of radical pairs with instantaneously changing spin Hamiltonian. I. General theory and kinematic approximation, A.B. Doktorov, S.A. Mikhailov and P.A. Purtov 160 (1992) 223
Theory of geminate recombination of radical pairs with instantaneously changing spin-Hamiltonian. II. Method of summation of re-encounter contributions, A.B. Doktorov, S.A. Mikhailov and P.A. Purtov 160 (1992) 239

Equilibrium statistical mechanics
Cluster structure in model electrolyte solutions, J.L.F. Abascal and P. Turq 153 (1991) 79
A dipolar chain model for the electrostatics of transmembrane ion channels, M.B. Partenskii, M. Cai and P.C. Jordan 153 (1991) 125
Doppler-free radio frequency lineshape theory for a three-level system with three allowed transitions in presence of an IR pump, S. Ghoshal and A. Datta 153 (1991) 161
Polyatomic fluids near solid surfaces: a weighted-density-functional approach, T.A. Cherepanova and A.V. Stekolnikov 154 (1991) 41
A dipolar chain model for the electrostatics of transmembrane ion channels, Chem. Phys. 153 (1991) 125–131. Erratum, M.B. Partenskii, M. Cai and P.C. Jordan 154 (1991) 197
The two-dimensional electrolytic solution in the hypernetted chain approximation, W. Chung and S.S. Mak 155 (1991) 19
Monte Carlo and mean field studies of a polyelectrolyte in salt solution, C.E. Woodward and B. Jönsson 155 (1991) 207
Spatial distribution of probes in a micelle: effects on the energy transfer time-resolved measurables, A.V. Barzykin 155 (1991) 221
Structure and dynamics of polar liquids: a molecular dynamics investigation of N,N-dimethyl formamide, S. Yashonath and C.N.R. Rao 155 (1991) 351
Zinc ion in water: intermolecular potential with approximate three-body correction and Monte Carlo simulation, Y.P. Yongyai, S. Kokpol and B.M. Rode 156 (1991) 403
Molecular dynamics simulation of superoxide interacting with superoxide dismutase, J. Shen and J.A. McCammon 158 (1991) 191
Comparison of lattice Monte Carlo dynamics and Brownian dynamics folding pathways of α-helical hairpins, A. Rey and J. Skolnick 158 (1991) 199
Theory of long time peptide dynamics: test of various reduced descriptions and role of internal variables, Y. Hu, G.R. Fleming, K.F. Freed and A. Perico 158 (1991) 395
A validity test of the WCA perturbation theory for two-dimensional Lennard-Jones fluids, F. Cuadros and A. Mulero 160 (1992) 375

Statistical mechanics of stationary states
Velocity dependence of friction, S.-B. Zhu, S. Singh, J. Lee and G.W. Robinson 152 (1991) 221
Generalized Einstein relations for ions in molecular gases, A.D. Koutselos and E.A. Mason 153 (1991) 351

Material properties of low-dimensional charge-transfer salts. II. Mode-softening, Peierls transitions and van Hove singularities, M.C. Böhm 155 (1991) 49
Three-time autocorrelation function of the power associated with a Gaussian random process, L. Song and J.M. Schurr 155 (1991) 63
Computer simulation of partially diffusion-controlled reactions, M.A. López-Quintela and M.C. Buján-Núñez 157 (1991) 307
Interaction between two chemical reactions in gases. The nonequilibrium effects from the Boltzmann and Fokker–Planck equations within a Lorentz gas model, A.S. Cukrowski, A.L. Kawczyński, J. Popielawski, W. Stiller and R. Schmidt 159 (1992) 39
Chemical potential, partial enthalpy and partial volume of mixtures by *NPT* molecular dynamics, D.M. Heyes 159 (1992) 149
Experimental and theoretical investigation of the reaction $CF_3+NO+M\rightarrow CF_3NO+M$ from 0.5 to 12 Torr and from 253 to 373 K, J. Masanet, F. Caralp, L. Ley and R. Lesclaux 160 (1992) 383

Non-equilibrium thermodynamic and hydrodynamic theories
Generalized Langevin model for molecular dynamics of an activated reaction in solution, I. Benjamin, L.L. Lee, Y.S. Li, A. Liu and K.R. Wilson 152 (1991) 1
The probability of non-adiabatic electron transfer as a function of friction, A.I. Burshtein and A.A. Zharikov 152 (1991) 23
Solvent effect on activated rate processes: on the validity of the GLE approach, G. Tarjus and D. Kivelson 152 (1991) 153
Chemical reaction rates and solvation dynamics in electrolyte solutions: ion atmosphere friction, G. van der Zwan and J.T. Hynes 152 (1991) 169
Outer-sphere electron-transfer reactions in model molecular solvents: the mean spherical approximation, Y. Zhou, H.L. Friedman and G. Stell 152 (1991) 185
Ion solvation dynamics in an interaction-site model solvent, F.O. Raineri, Y. Zhou, H.L. Friedman and G. Stell 152 (1991) 201
Heavy ions in mixtures of light gases: Fokker–Planck equation and its solution, L. Ferrari 153 (1991) 115
Effects of solvent viscoelasticity in the solvation dynamics of an ion in a dense dipolar liquid, A. Chandra and B. Bagchi 156 (1991) 323
Theory of diffusion-influenced fluorescence quenching: dependence of the Stern–Volmer curve on light intensity, S. Lee, M. Yang, K.J. Shin, K.Y. Choo and D. Lee 156 (1991) 339
Activated rate processes in the multidimensional case. Consideration of recrossings in the multidimensional Kramers problem with anisotropic friction, A.M. Berezhkovskii and V.Yu. Zitserman 157 (1991) 141
Dissociation rate and $N(^4S)$ atom concentrations in a N_2 glow-discharge, J. Loureiro 157 (1991) 157
Dynamics of charge transfer chemical reactions in a polar medium within the scope of the Born–Kirkwood–Onsager model, M.V. Basilevsky and G.E. Chudinov 157 (1991) 327
The configuration interaction theory for charge transfer chemical processes in a polar solvent, M.V. Basilevsky and G.E. Chudinov 157 (1991) 345
Driven damped harmonic oscillators perturbed by the parity operator, P. Blaise, M. Giry and O. Henri-Rousseau 159 (1992) 169

Ab initio schemes for stationary properties
Theoretical study of the spectroscopy of Al_2^+, M. Rosi, C.W. Bauschlicher Jr. and S.R. Langhoff 151 (1991) 1
Electronic structure of linear form of OCuO, Y. Mochizuki, K. Tanaka and H. Kashiwagi 151 (1991) 11

Ab initio molecular orbital treatment of hydroxylamine–X^+–water and hydroxylamine–X^+–ammonia (X=H, Li) clusters, M. Alcamí, O. Mó and M. Yáñez 151 (1991) 21
Calculation of the vibrational frequency and line strength versus applied field of carbon monoxide, J.L. Andrés, M. Duran, A. Lledós and J. Bertrán 151 (1991) 37
Rotation–vibration energies of FHF^- and $ClHCl^-$ from high-level correlated calculations of potential energy surfaces, V. Špirko, A. Čejchan and G.H.F. Diercksen 151 (1991) 45
Ab initio SCF study on $LiClO_4$ and Li_2SO_4 molecules: geometries and vibrational frequencies, F. Ramondo, L. Bencivenni, R. Caminiti and C. Sadun 151 (1991) 179
The H_2O_2–NO_2^- and $H_2NO_4^-$ isomers of the nitrate anion–water complex, M. Shen, Y. Xie, H.F. Schaefer III and C.A. Deakyne 151 (1991) 187
Theoretical study of the electronic states of BeLi and Be_2^+, I. Fischer, V.E. Bondybey, P. Rosmus and H.-J. Werner 151 (1991) 295
Jahn–Teller effect and dissociation from the ground state of CF_4^+, J.M. García de la Vega and E. San Fabián 151 (1991) 335
MRCI potential energy functions for the charge transfer reactions $H^+ + HCl$ $(X^1\Sigma^+) \rightarrow H + HCl^+$ $(X^2\Pi_i, A^2\Sigma^+)$, Th. Glenewinkel-Meyer, Ch. Ottinger, P. Rosmus and H.-J. Werner 152 (1991) 409
Theoretical study of the spectroscopy of the alkali oxides LiO, NaO, and KO, S.R. Langhoff, H. Partridge and C.W. Bauschlicher Jr. 153 (1991) 1
Ab initio calculations on the one- and two-photon electronic transitions of cyclopentadiene, spirononateraene, 1,4-cyclo-hexadiene, Dewar benzene, norbornadiene, and barrelene, V. Galasso 153 (1991) 13
Observable-dedicated molecular orbitals. I. Method and illustrations, J. Miralles, R. Caballol and J.-P. Malrieu 153 (1991) 25
Acrylonitrile versus allyl cyanide: the role of electronic conjugation in high electric field condition, M. Raynaud, C. Reynaud, Y. Ellinger, G. Hennico and J. Delhalle 153 (1991) 39
Vibrational structure of the solvated glycine zwitterion, J.S. Alper, H. Dothe and D.F. Coker 153 (1991) 51
A quantum chemical study on the alternative mechanisms of the thermal cis–trans isomerization of streptocyanines, T. Krossner and F. Dietz 153 (1991) 63
The electronic states of the azines. IV. Pyrazine, studied by VUV absorption, near-threshold electron energy-loss spectroscopy and ab initio multi-reference configuration interaction calculations, I.C. Walker and M.H. Palmer 153 (1991) 169
The magnetizability and *g*-factor surfaces of ammonia, S.P.A. Sauer, V. Špirko and J. Oddershede 153 (1991) 189
The structures and stability of the $Si_3H_6^{2+}$ dications. A theoretical study, T. Kudo and S. Nagase 153 (1991) 379
Bond formation between positively charged species. Non-adiabatic analysis and valence-bond model in the CO^{2+} case, N. Levasseur, Ph. Millie, P. Archirel and B. Levy 153 (1991) 387
Heteronuclear transition metal diatomics: the bonding and electronic structure of ScNi, YNi, ScPd and YPd, K. Faegri Jr. and C.W. Bauschlicher Jr. 153 (1991) 399
The correlated molecular electrostatic potential and electric field of 2(1H)-pyrimidone and 2-hydroxypyrimidine, A. Leś and L. Adamowicz 153 (1991) 409
Calculation of excitation energies using quasidegenerate variational perturbation theory and multireference-averaged coupled-pair functional theory, M.A. Anderson and R.J. Cave 154 (1991) 1
Theoretical study of the electronic spectrum of ammonia: generalized oscillator strength calculations for the A–X transition, L. Chantranupong, G. Hirsch, R.J. Buenker, M. Kimura and M.A. Dillon 154 (1991) 13

Ab initio study of the infrared photoconversion in the water–hydrogen iodide system, Y. Hannachi, B. Silvi, J.P. Perchard and Y. Bouteiller 154 (1991) 23
An experimental and theoretical study of SF^{q+} ($q=1$–3) ions, K. Nagesha, V.R. Marathe and D. Mathur 154 (1991) 125
Potential curves and predissociation rates for the heavy species HBr^{2+} and DBr^{2+}, A. Banichevich, S.D. Peyerimhoff, B.A. Hess and M.C. van Hemert 154 (1991) 199
Calculation of the inner shell excitation spectra and estimation of the electron scattering and dissociative attachment resonance energies of SF_6, SO_2, SF_2O, SF_2O_2, SF_4, SF_4O and S_2F_{10}, J.A. Tossell 154 (1991) 211
Isomerization and unimolecular rearrangement channels of dithioformic acid, Y. Tao 154 (1991) 221
A theoretical study on the internal rotation and hyperfine structures of the ethyl radical (CH_3–CH_2), H.U. Suter and T.K. Ha 154 (1991) 227
Rotational spectrum and structure of the linear HCN–HCCH dimer, A.I. Jaman, T.C. Germann, H.S. Gutowsky, J.D. Augspurger and C.E. Dykstra 154 (1991) 281
Model potentials in numerical local density functional methods, G.L. Gutsev, V.K. Gryaznov and V.A. Nasluzov 154 (1991) 291
The generator coordinate Hartree–Fock method for molecular systems. Formalism and first applications to H_2, LiH and Li_2, H.F.M. da Costa, A.B.F. da Silva, J.R. Mohallem, A.M. Simas and M. Trsic 154 (1991) 379
A theoretical investigation of the hyperfine properties of normal and anomalous muonium in elemental semiconductors: diamond, silicon and germanium, M. Casarin, G. Granozzi, E. Tondello and A. Vittadini 154 (1991) 385
Quantum kinetic energy operator for a group of particles in terms of scalar basic rotational invariant coordinates derived from a generalized Jacobi vector (GJV) description. III. A metric tensors approach, J.P. Leroy, H. Rabitz and R. Wallace 154 (1991) 395
Core–valence correlation effects on some Cu clusters, H. Åkeby and L.G.M. Pettersson 155 (1991) 197
Localization and correlation corrections in electronic interactions through single bonded hydrocarbon spacers, M. Braga, A. Broo and S. Larsson 156 (1991) 1
On the elastic properties of lithium, sodium and potassium oxide. An ab initio study, R. Dovesi, C. Roetti, C. Freyria-Fava, M. Prencipe and V.R. Saunders 156 (1991) 11
The vibrational spectra of the monohalogenated cyclopropanes: ab initio calculations and an experimental study of fluorocyclopropane, C. Kaupert, H. Heydtmann and W. Thiel 156 (1991) 85
Nodal configurations and many-body energies in Li_3^{3+}, F_3^{3-}, $Li_2^{2+}F^-$ and $Li^+F_2^{2-}$ ions at crystal and cluster geometries, A.S. Shalabi 156 (1991) 359
Nuclear quadrupole coupling constants of rovibrational levels of all isotopic species of BH^+ in their $X\,^2\Sigma^+$ and $B'\,^2\Sigma^+$ states, J. Vojtík, L. Češpiva, I. Paidarová and J. Šavrda 156 (1991) 369
A theoretical study of the chemisorption of methane on a Ni(100) surface, O. Swang, K. Faegri Jr., O. Gropen, U. Wahlgren and P. Siegbahn 156 (1991) 379
Theoretical study of optical excitations of linear C_4^-, L. Adamowicz 156 (1991) 387
Ab initio calculation of the second virial coefficient of neon and the potential energy curve of Ne_2, R. Eggenberger, S. Gerber, H. Huber and D. Searles 156 (1991) 395
The structure and stability of Cl_n^- clusters, $n=2$–7, G.L. Gutsev 156 (1991) 427
Adiabatic calculations and properties of the He_2^+ molecular ion, J. Ackermann and H. Hogreve 157 (1991) 75
Ab initio quantum-chemical study of the unimolecular pyrolysis mechanisms of fluoroformic and chloroformic acid, J.S. Francisco and W.A. Ghoul 157 (1991) 89
Singlet–triplet energy component differences in homonuclear diatomics: a multi-reference configuration interaction study of Hund's rule, K.V. Darvesh, P.D. Fricker and R.J. Boyd 157 (1991) 99

Ab initio calculation of phosphorus NMR chemical shifts in the gauge including atomic orbital method, D.B. Chesnut and B.E. Rusiloski 157 (1991) 105
Transition probabilities for the $B\,^1\Delta_g$–$A\,^1\Pi_u$ and $B'\,^1\Sigma_g^+$–$A\,^1\Pi_u$ infrared bands of C_2. An ab initio study, P.J. Bruna and J.S. Wright 157 (1991) 111
Interaction potentials in rare gas–halide ion systems, V. Kellö and A.J. Sadlej 157 (1991) 123
The electronic states of the azines. V. Pyridazine, studied by VUV absorption, near threshold electron energy-loss spectroscopy and ab initio multi-reference configuration interaction calculations, M.H. Palmer and I.C. Walker 157 (1991) 187
Ring-puckering and internal rotation barriers in N,N′-dimethylethyleneurea, J.C. Otero, J.I. Marcos, E. López-Cantarero and A. Chacón 157 (1991) 201
Ground state electric properties of NaH, G.H.F. Diercksen and A.J. Sadlej 158 (1991) 9
Electric properties of ionic diatoms: BeO, G.H.F. Diercksen, A.J. Sadlej and M. Urban 158 (1991) 19
The structure and stability of S_2F_{10} and S_2F_{11} and their anions, G.L. Gutsev 158 (1991) 33
Ab initio calculation of anharmonic force fields for the methyl, silyl, germyl, and stannyl halides, W. Schneider and W. Thiel 159 (1992) 49
From cluster to crystal: ab initio calculations of the OH^- frequency in lithium hydroxide monohydrate, K. Hermansson 159 (1992) 67
Variational approach to continuum orbitals in a spline basis: an application to H_2^+ photoionization, M. Brosolo and P. Decleva 159 (1992) 185
Comparative study on the structures and energies of the SiX_3, GeX_3 and SnX_3 series of radicals (X=H, F, Cl), J. Moc, J.M. Rudziński and H. Ratajczak 159 (1992) 197
Solvatochromatic shifts studied by multi-configuration self-consistent reaction field theory. Application to azabenzenes, H. Ågren, S. Knuts, K.V. Mikkelsen and H.J.Aa. Jensen 159 (1992) 211
Ab-initio multiple reference double-excitation configuration-interaction ground and excited state potential curves for the H_2N–NO_2 decomposition in nitramine, S. Roszak and J.J. Kaufman 160 (1992) 1
Ab initio study of the vibrational structure of the $X\,^2A_1$ and $A\,^2B_1$ electronic states of CH_2^+, W. Reuter and S.D. Peyerimhoff 160 (1992) 11
The Pariser–Parr–Pople model for trans-polyenes. I. Ab initio and semiempirical study of the bond alternation in trans-butadiene, W. Förner 160 (1992) 173
Structural and spectral consequences of ion-pairing. VI. $BO_2^-Li^+$ and $BO_2^-Na^+$, J.S. Francisco and I.H. Williams 160 (1992) 255

Computational and simulation methods

Rotation–vibration energies of FHF^- and $ClHCl^-$ from high-level correlated calculations of potential energy surfaces, V. Špirko, A. Čejchan and G.H.F. Diercksen 151 (1991) 45
Model studies on femtosecond time-resolved ionization spectroscopy of excited-state vibrational dynamics and vibronic coupling, M. Seel and W. Domcke 151 (1991) 59
Optical potentials by the complex coordinate method, N. Rom, N. Lipkin and N. Moiseyev 151 (1991) 199
Polar phonons in SO_2 single crystal, A. Tafi, P. Procacci, E. Castellucci and P.R. Salvi 151 (1991) 205
Theoretical infrared spectra of large carbon clusters, D. Bakowies and W. Thiel 151 (1991) 309
EPR investigation of chromium(III) complexes: analysis of their frozen solution and magnetically dilute powder spectra, R.P. Bonomo, A.J. Di Bilio and F. Riggi 151 (1991) 323
Generalized Langevin model for molecular dynamics of an activated reaction in solution, I. Benjamin, L.L. Lee, Y.S. Li, A. Liu and K.R. Wilson 152 (1991) 1
An exact theory of friction for reactive collisions in a solvent using an interaction representation, D.M. Charutz and R.D. Levine 152 (1991) 31

Solvent cage effects and chemical dynamics in liquids, F. Patron and S.A. Adelman 152 (1991) 121
Vibrational structure of the solvated glycine zwitterion, J.S. Alper, H. Dothe and D.F. Coker 153 (1991) 51
A quantum chemical study on the alternative mechanisms of the thermal cis–trans isomerization of streptocyanines, T. Krossner and F. Dietz 153 (1991) 63
Trajectory capture rate coefficients for ion–quadrupolar molecule reactions, I. Mendaš and P. Milutinović 153 (1991) 73
Cluster structure in model electrolyte solutions, J.L.F. Abascal and P. Turq 153 (1991) 79
The correlated molecular electrostatic potential and electric field of 2(1H)-pyrimidone and 2-hydroxypyrimidine, A. Leś and L. Adamowicz 153 (1991) 409
Theoretical study of the reaction of OH with HNO, M.R. Soto, M. Page and M.L. McKee 153 (1991) 415
Electron spin exchange in micellized radical pairs. I. ^{13}C low field chemically induced dynamic nuclear polarization (CIDNP) and ^{13}C radio frequency stimulated nuclear polarization (SNP), I.A. Shkrob, V.F. Tarasov and E.G. Bagryanskaya 153 (1991) 427
Electron spin exchange in micellized radical pairs. II. Magnetic field and magnetic isotope effects in multinuclear pairs, I.A. Shkrob, V.F. Tarasov and A.L. Buchachenko 153 (1991) 443
Conformational dependence of the quadratic hyperpolarisabilities of a series of push–pull diaryl acetylenes: an experimental and computational investigation, M. Barzoukas, A. Fort, G. Klein, A. Boeglin, C. Serbutoviez, L. Oswald and J.F. Nicoud 153 (1991) 457
Connecting level statistics and reaction dynamics: mode selective decay of resonant states for HXXH-type molecules, B. Hartke and W. Karrlein 154 (1991) 63
Quasiclassical trajectory study of the two channels of the F+ICl system: effect of the collisional energy, I. Urrecha, I. Serna and J. Iturbe 154 (1991) 85
Anomalous magnetic effects. The role of association in the recombination of singlet radical pairs in liquids, N.V. Shokhirev, E.C. Korolenko, M.B. Taraban and T.V. Leshina 154 (1991) 237
Lattice dynamics of the orthorhombic phase of $KClO_4$: Ewald's method in molecular coordinates, G.F. Signorini, R. Righini and V. Schettino 154 (1991) 245
On the solution of the Debye–Smoluchowski equation with a Coulomb potential. III. The case of a Boltzmann initial distribution and a perfectly absorbing sink, S.D. Traytak 154 (1991) 263
On the validity of the RWA for steady state and temporal populations of molecular states involved in IR multi-photon excitations, S. Nakai and W.J. Meath 154 (1991) 349
Motion and geminal recombination of charged carriers in highly anisotropic three-dimensional systems (Onsager theory), G.A. Vinogradov, V.N. Likhachev and A.A. Ovchinnikov 154 (1991) 367
The generator coordinate Hartree–Fock method for molecular systems. Formalism and first applications to H_2, LiH and Li_2, H.F.M. da Costa, A.B.F. da Silva, J.R. Mohallem, A.M. Simas and M. Trsic 154 (1991) 379
On the disordered distribution of defects in transpolyacetylene, F.C. Lavarda, D.A. dos Santos, D.S. Galvão and B. Laks 155 (1991) 1
Chiral discrimination: a model for the interaction between an helicoidal system and an amino acid molecule, E. Alvira, J. Breton, J. Plata and C. Girardet 155 (1991) 7
The two-dimensional electrolytic solution in the hypernetted chain approximation, W. Chung and S.S. Mak 155 (1991) 19
Material properties of low-dimensional charge-transfer salts. I. Charge fluctuations in systems with stronger electronic correlations, M.C. Böhm and A. Staib 155 (1991) 27
Hole pairing on oxygen sites in high-T_c copper–oxide superconductors induced by an effective exchange interaction: a theoretical and numerical investigation on planar lattices, A. Ferretti and A. Lami 155 (1991) 179

Potential of mean force by constrained molecular dynamics: a sodium chloride ion-pair in water, E. Guàrdia, R. Rey and J.A. Padró 155 (1991) 187
Core–valence correlation effects on some Cu clusters, H. Åkeby and L.G.M. Pettersson 155 (1991) 197
Monte Carlo and mean field studies of a polyelectrolyte in salt solution, C.E. Woodward and B. Jönsson 155 (1991) 207
Structure and dynamics of polar liquids: a molecular dynamics investigation of N,N-dimethyl formamide, S. Yashonath and C.N.R. Rao 155 (1991) 351
New Monte Carlo simulations of many-particle stochastic dynamics: growth of correlations and local self-ordering during annihilation of like particles, R. Brown and N.A. Efremov 155 (1991) 357
A vibrational study of the CD_3H molecule in the curvilinear formulation, C. Iung and C. Leforestier 155 (1991) 369
Experimental and theoretical study of the N_{1s} and C_{1s} shake-up satellites in pyridine and aniline, M.P. Keane, A. Naves de Brito, N. Correia, S. Svensson and S. Lunell 155 (1991) 379
A model description of charge carrier transport phenomena in organic molecular crystals. II. Perylene, E.A. Silinsh, G.A. Shlihta and A.J. Jurgis 155 (1991) 389
On the elastic properties of lithium, sodium and potassium oxide. An ab initio study, R. Dovesi, C. Roetti, C. Freyria-Fava, M. Prencipe and V.R. Saunders 156 (1991) 11
Scaling the WCA reference system for two-dimensional Lennard-Jones fluids, F. Cuadros and A. Mulero 156 (1991) 33
Simulation of the unstable dynamics of excitable biomembranes: properties of a cyclic electrochemical gating mechanism, K.D. Schulze 156 (1991) 43
Theoretical study of multiple-scattering effects in the X-ray absorption spectra of iron-porphyrins, F. Bohr and M.F. Ruiz-López 156 (1991) 55
The influence of physisorption and the Eley–Rideal mechanism on a surface reaction: $CO+O_2$, J. Mai and W. von Niessen 156 (1991) 63
Molecular dynamics simulation of crystalline imidazole, S. Besnainou, G. Cardini and D.A. Dows 156 (1991) 71
Isomer-specific radiative lifetimes of molecular heteroclusters, D. Bahatt, U. Even, E. Shalev, N. Ben-Horin and J. Jortner 156 (1991) 223
Vibrational relaxation of glyoxal in collisions with He and Ar, G.-J. Kroes and R.P.H. Rettschnick 156 (1991) 293
Theoretical study of optical excitations of linear C_4^-, L. Adamowicz 156 (1991) 387
Ab initio calculation of the second virial coefficient of neon and the potential energy curve of Ne_2, R. Eggenberger, S. Gerber, H. Huber and D. Searles 156 (1991) 395
Zinc ion in water: intermolecular potential with approximate three-body correction and Monte Carlo simulation, Y.P. Yongyai, S. Kokpol and B.M. Rode 156 (1991) 403
A combining rule calculation of the van der Waals potentials of the rare-gas hydrides, K.T. Tang and J.P. Toennies 156 (1991) 413
The structure and stability of Cl_n^- clusters, $n=2$–7, G.L. Gutsev 156 (1991) 427
Test-particle model potentials for hydrogen-bonded complexes: complexes formed from HCN, HF, H_2O, NH_3, $HCONH_2$, $HCONHCH_3$, guanine and cytosine, K.P. Sagarik, V. Pongpituk, S. Chaiyapongs and P. Sisot 156 (1991) 439
Intramolecular dynamics of the C_4H_8NH radical cation. An application of the anisotropic exchange theory for powder ESR lineshapes, L. Sjöqvist, N.P. Benetis, A. Lund and J. Maruani 156 (1991) 457
Theory and simulation of optically induced line shifts in NMR, M.W. Evans 157 (1991) 1

Construction of bound-state potential energy curves of diatomic molecules from spectroscopic data, C.G. Diaz, F.M. Fernández and E.A. Castro 157 (1991) 35
Quantumchemical electronegativity and hardness indices for bonded atoms, L. Komorowski and J. Lipiński 157 (1991) 45
Specific heat from an unsymmetrical double well potential, I.D. Feranchuk, A.P. Ulyanenkov and V.S. Kuz'min 157 (1991) 61
Modified version of the trajectory surface leaking method for dynamical calculations on autoionizing atom–diatom collision systems, J. Vojtík and I. Paidarová 157 (1991) 67
Adiabatic calculations and properties of the He_2^+ molecular ion, J. Ackermann and H. Hogreve 157 (1991) 75
Computer simulation of partially diffusion-controlled reactions, M.A. López-Quintela and M.C. Buján-Núñez 157 (1991) 307
General numerical solution to the time-dependent master equation for non-steady-state reactions: application to the photoinitiated isomerization of cycloheptatriene to toluene, R.L. Jackson 157 (1991) 315
The structure and stability of S_2F_{10} and S_2F_{11} and their anions, G.L. Gutsev 158 (1991) 33
Ab initio study on the coordination structures of $M^+XY_3^-$ and $M^+XY_4^-$ ion pairs, F. Ramondo, L. Bencivenni and V. Di Martino 158 (1991) 41
The condensed phases of pyrazine: a test of the Williams–Weller intermolecular potential, Z. Gamba 158 (1991) 59
Molecular dynamics simulations of water–methanol mixtures, G. Pálinkás, E. Hawlicka and K. Heinzinger 158 (1991) 65
Molecular dynamics simulation of superoxide interacting with superoxide dismutase, J. Shen and J.A. McCammon 158 (1991) 191
Comparison of lattice Monte Carlo dynamics and Brownian dynamics folding pathways of α-helical hairpins, A. Rey and J. Skolnick 158 (1991) 199
Quantum simulation of conformation reorganization in the electron transfer reactions of tuna cytochrome c, C. Zheng, J.A. McCammon and P.G. Wolynes 158 (1991) 261
Stabilization of α-helical secondary structure during high-temperature molecular-dynamics simulations of α-lactalbumin, P. Fan, D. Kominos, D.B. Kitchen, R.M. Levy and J. Baum 158 (1991) 295
The dynamics of the primary event in rhodopsins revisited, A. Warshel, Z.T. Chu and J.-K. Hwang 158 (1991) 303
The effects of environment and hydration on protein dynamics: a simulation study of myoglobin, P.J. Steinbach, R.J. Loncharich and B.R. Brooks 158 (1991) 383
Coupling of protein motion to electron transfer: molecular dynamics and stochastic quantum mechanics study of photosynthetic reaction centers, K. Schulten and M. Tesch 158 (1991) 421
The effects of solvent on the conformation and the collective motions of protein: normal mode analysis and molecular dynamics simulations of melittin in water and in vacuum, A. Kitao, F. Hirata and N. Gō 158 (1991) 447
Far-infrared perturbation of electron tunneling in reaction centers?, R.H. Austin, M.K. Hong, C. Moser and J. Plombon 158 (1991) 473
A molecular dynamics simulation of the C-terminal fragment of the L7/L12 ribosomal protein in solution, V. Daggett and M. Levitt 158 (1991) 501
MO LCAO analysis of the vibronic instability of the $CuCl_5^{3-}$ trigonal bipyramidal configuration. Critical view on the angular overlap model in vibronic problems, V.Z. Polinger, N.N. Gorinchoi and I.B. Bersuker 159 (1992) 75

The radial distribution function for two-dimensional Lennard-Jones fluids: computer simulation results, F. Cuadros and A. Mulero 159 (1992) 89
A semiclassical simulation for tunneling dynamics of malonaldehyde and hydrogenoxalate anion, E. Bosch, M. Moreno and J.M. Lluch 159 (1992) 99
Quasiclassical trajectory study of the effect of reactant rotation on the reaction $B^+ + HD \rightarrow BH^+(BD^+) + D(H)$, V. Klimo, J. Urban and J. Tiňo 159 (1992) 141
Chemical potential, partial enthalpy and partial volume of mixtures by *NPT* molecular dynamics, D.M. Heyes 159 (1992) 149
Site effects in spectra of matrix-isolated diatomic molecules: a modelling approach, M. Winter, K. Seranski and U. Schurath 159 (1992) 235
The dynamics of dressed variables, D.M. Charutz and R.D. Levine 159 (1992) 321
Assessment of Gaussian-weighted angular resolution functions in the comparison of quantum-mechanically calculated electron momentum distributions with experiment, P. Duffy, M.E. Casida, C.E. Brion and D.P. Chong 159 (1992) 347
A theoretical investigation of the electronic structure, hyperfine properties and binding energies of muonium centres in cuprous chloride, M. Casarin, G. Granozzi, E. Tondello and A. Vittadini 159 (1992) 365
Ab-initio multiple reference double-excitation configuration-interaction ground and excited state potential curves for the $H_2N–NO_2$ decomposition in nitramine, S. Roszak and J.J. Kaufman 160 (1992) 1
Methyl tunnelling in solid diacetyl, A.M. Alsanoosi and A.J. Horsewill 160 (1992) 25
Test of effective pair potential models by molecular dynamics simulation on liquid OCS, J. Samios, H. Stassen and T. Dorfmüller 160 (1992) 33
Quantum-chemical calculations of the hydration energies of organic cations and anions in the framework of a continuum solvent approximation, G.E. Chudinov, D.V. Napolov and M.V. Basilevsky 160 (1992) 41
Intramolecular charge transfer and trans–cis isomerization of the DCM styrene dye in polar solvents. A CS INDO MRCI study, S. Marguet, J.C. Mialocq, P. Millie, G. Berthier and F. Momicchioli 160 (1992) 265
Computational experiments on the intramolecular energy flow in macromolecules, B.G. Sumpter and D.W. Noid 160 (1992) 393
Comparative studies of the underlying local order corresponding to different radial distribution functions of disordered materials, G. Tóth and L. Pusztai 160 (1992) 405
Local density functional study of the structural and electronic properties of C_{60} and XC_{60} (X=K,Rb,Cs), L. Ye, A.J. Freeman and B. Delley 160 (1992) 415

Molecular dynamics and scattering theory

Symmetry and magnetic vibrational circular dichroism spectra of a doubly degenerate vibration and its combinations with non-degenerate vibrational modes, M. Pawlikowski and O. Sonnich Mortensen 151 (1991) 73
A multisurface classical trajectory study of the dynamics of the reaction $O(^1D_2) + H_2 \rightarrow OH(v', J', \Theta') + H$ using the diatomics in molecules method, P.J. Kuntz, B.I. Niefer and J.J. Sloan 151 (1991) 77
A classical study on the vibrational motion of a diatomic molecule in a collisional vibronic excitation, R.F.M. Lobo and A.M.C. Moutinho 151 (1991) 95
Optical potentials by the complex coordinate method, N. Rom, N. Lipkin and N. Moiseyev 151 (1991) 199
Model study of the effect of anisotropy on the differential cross section for atom–molecule scattering: the double rainbows, R. Düren, R.K.B. Helbing and S. Milošević 151 (1991) 287

An exact theory of friction for reactive collisions in a solvent using an interaction representation, D.M. Charutz and R.D. Levine 152 (1991) 31
Solvent dynamical effects in electron transfer: the solvent inertial limit and the predicted influence of quantum effects, G.E. McManis, A. Gochev and M.J. Weaver 152 (1991) 107
Net CIDNP in geminate radical pair recombination in viscous liquids. Comparison of theory and experiment for high magnetic fields, A.I. Shushin 152 (1991) 133
Velocity dependence of friction, S.-B. Zhu, S. Singh, J. Lee and G.W. Robinson 152 (1991) 221
Symmetry breaking in thermally activated NH_4 rotation studied by NMR level crossing spectroscopy, S. Clough, A.J. Horsewill, M.R. Johnson, M.A. Mohammed and T. Newton 152 (1991) 343
Vibrational structure of the solvated glycine zwitterion, J.S. Alper, H. Dothe and D.F. Coker 153 (1991) 51
Trajectory capture rate coefficients for ion–quadrupolar molecule reactions, I. Mendaš and P. Milutinović 153 (1991) 73
An extended diatomics-in-molecules model for NH_2^+, R. Polák 153 (1991) 91
Relaxation cross sections for transfer of rotational angular momentum in a semiclassical approximation, A.V. Storozhev and M.L. Strekalov 153 (1991) 99
Quantum effects in competitive unimolecular reactions, F. Remacle, M. Desouter-Lecomte and J.C. Lorquet 153 (1991) 201
Estimation of the integral cross section for dissociative excitation of F_2 by electron impact, D.C. Cartwright, P.J. Hay and S. Trajmar 153 (1991) 219
Periodic orbits and quantum localization in the van der Waals systems CO–Ar, L. Zachilas and S.C. Farantos 154 (1991) 55
Connecting level statistics and reaction dynamics: mode selective decay of resonant states for HXXH-type molecules, B. Hartke and W. Karrlein 154 (1991) 63
Quasiclassical trajectory study of the two channels of the F+ICl system: effect of the collisional energy, I. Urrecha, I. Serna and J. Iturbe 154 (1991) 85
Quantum kinetic energy operator for a group of particles in terms of scalar basic rotational invariant coordinates derived from a generalized Jacobi vector (GJV) description. III. A metric tensors approach, J.P. Leroy, H. Rabitz and R. Wallace 154 (1991) 395
Low-temperature chemical reactions. Effect of symmetrically coupled vibrations in collinear exchange reactions, V.A. Benderskii, V.I. Goldanskii and D.E. Makarov 154 (1991) 407
Shape resonances in photoionizations of cyanoacetylene. Experimental and theoretical investigations of the $\tilde{X}\,^2\Pi$, $\tilde{A}\,^2\Sigma$ and $\tilde{B}\,^2\Pi$ ionizations up to a photon energy of 28 eV, J. Kreile, H.-D. Kurland, W. Seibel and A. Schweig 155 (1991) 99
Symmetry and vibronic coupling: the stereochemistry and the ground state potential surface of Cu^{2+} in five-coordination, D. Reinen and M. Atanasov 155 (1991) 157
The phase space moment method for studying intramolecular vibrational energy redistribution, G. Huacai and J. Fenglin 155 (1991) 345
Molecular dynamics simulation of crystalline imidazole, S. Besnainou, G. Cardini and D.A. Dows 156 (1991) 71
New mechanism for the vibrational mode-specific proton-transfer reaction $NH_3^+(v)+NH_3 \rightarrow NH_2+NH_4^+$, A. Tachibana, T. Suzuki, N. Yoshida, Y. Teramoto and T. Yamabe 156 (1991) 79
Real-time dynamics of vibrational predissociation in anthracene–Ar_n ($n=1,2,3$), A. Heikal, L. Bañares, D.H. Semmes and A.H. Zewail 156 (1991) 231
Vibrational relaxation of glyoxal in collisions with He and Ar, G.-J. Kroes and R.P.H. Rettschnick 156 (1991) 293
A combining rule calculation of the van der Waals potentials of the rare-gas hydrides, K.T. Tang and J.P. Toennies 156 (1991) 413

Modified version of the trajectory surface leaking method for dynamical calculations on autoionizing atom–diatom collision systems, J. Vojtík and I. Paidarová 157 (1991) 67
On the critical scattering phenomena of a nonpolar fluid composed of chiral molecules, E.-K. Lee, D.J. Lee and S.K. Kim 157 (1991) 135
Variational approach to quantum dynamics: a simple application to molecular photodissociation, G.P. Arrighini, N. Durante and C. Guidotti 157 (1991) 365
Molecular dynamics simulations of water–methanol mixtures, G. Pálinkás, E. Hawlicka and K. Heinzinger 158 (1991) 65
The He–N_2 interaction revisited: a comparison of measured and computed differential cross sections, F.A. Gianturco, A. Palma and N. Sanna 158 (1991) 77
Angular momentum and rotational energy relaxation in N_2–N_2 collisions calculated from coherent and stimulated Raman spectroscopy data, S. Temkin, J.M. Thuet, L. Bonamy, J. Bonamy and D. Robert 158 (1991) 89
Molecular dynamics study of the photodissocation of carbon monoxide from myoglobin: ligand dynamics in the first 10 ps, J.E. Straub and M. Karplus 158 (1991) 221
Fluorescence and molecular dynamics study of the internal motion of the buried tryptophan in bacteriophage T4 lysozyme: effects of temperature and alteration of nonbonded networks, D.L. Harris and B.S. Hudson 158 (1991) 353
The effects of environment and hydration on protein dynamics: a simulation study of myoglobin, P.J. Steinbach, R.J. Loncharich and B.R. Brooks 158 (1991) 383
Far-infrared perturbation of electron tunneling in reaction centers?, R.H. Austin, M.K. Hong, C. Moser and J. Plombon 158 (1991) 473
Dynamics of the hydrate and amide groups of crystalline ribonuclease and lysozyme, M.G. Usha, J. Speyer and R.J. Wittebort 158 (1991) 487
A molecular dynamics simulation of the C-terminal fragment of the L7/L12 ribosomal protein in solution, V. Daggett and M. Levitt 158 (1991) 501
The radial distribution function for two-dimensional Lennard-Jones fluids: computer simulation results, F. Cuadros and A. Mulero 159 (1992) 89
A semiclassical simulation for tunneling dynamics of malonaldehyde and hydrogenoxalate anion, E. Bosch, M. Moreno and J.M. Lluch 159 (1992) 99
Quantum-classical reaction path model for chemical reactions. IV. The reaction $Cl^- + CH_3Cl \rightarrow ClCH_3 + Cl^-$, G.D. Billing 159 (1992) 109
Quasiclassical trajectory study of the effect of reactant rotation on the reaction $B^+ + HD \rightarrow BH^+(BD^+) + D(H)$, V. Klimo, J. Urban and J. Tiňo 159 (1992) 141
Variational approach to continuum orbitals in a spline basis: an application to H_2^+ photoionization, M. Brosolo and P. Decleva 159 (1992) 185
Time-dependent calculation of the energy resolved state-to-state transition probabilities for three-atom exchange reactions, M. Monnerville, P. Halvick and J.C. Rayez 159 (1992) 227
The importance of periodic orbits in analysing photodissociation resonances: the O_3 case, S.C. Farantos 159 (1992) 329
Energy transfer distributions for classical, collinear atom–diatom collisions, N. Snider 159 (1992) 339
A weak-mode representation of floppy molecules. I. Potential energy, C. Saint-Espès, X. Chapuisat and F. Schneider 159 (1992) 377
A weak-mode representation of floppy molecules. II. Kinetic energy and total Hamiltonian matrix, X. Chapuisat and C. Saint-Espès 159 (1992) 391
Master equation for site distributions describing barrier crossing in the presence of anisotropic diffusion, G.J. Moro 159 (1992) 421

Lie algebraic approach to scattering of molecules from a solid surface, S. Lin, X. Yi and L. Cai 160 (1992) 163
The Pariser–Parr–Pople model for trans-polyenes. II. Parametrization and ground state dynamics, W. Förner 160 (1992) 189
Generalized golden rule approach to the H-transfer problem. II. Application to a photochemical reaction, L. Lavtchieva and Z. Smedarchina 160 (1992) 211
A validity test of the WCA perturbation theory for two-dimensional Lennard-Jones fluids, F. Cuadros and A. Mulero 160 (1992) 375
Computational experiments on the intramolecular energy flow in macromolecules, B.G. Sumpter and D.W. Noid 160 (1992) 393

Experimental

Magnetic resonances

Triplet electron–proton cross-polarization by satisfying a modified Hartmann–Hahn condition, R.H. Fritsch, H. Brunner and K.H. Hausser 151 (1991) 261
Degenerate triplet spin exchange in liquid solution studied by pulse NMR, J. Burri and H. Fischer 151 (1991) 279
EPR investigation of chromium(III) complexes: analysis of their frozen solution and magnetically dilute powder spectra, R.P. Bonomo, A.J. Di Bilio and F. Riggi 151 (1991) 323
Net CIDNP in geminate radical pair recombination in viscous liquids. Comparison of theory and experiment for high magnetic fields, A.I. Shushin 152 (1991) 133
FIR LMR spectra of FO_2: some classic examples of level anticrossing resonances, U. Bley, P.B. Davies, M. Grantz, T.J. Sears and F. Temps 152 (1991) 281
A Zeeman level crossing study of the symmetry of the potential hindering the torsional oscillator CH_3, W.T. Sobol, I.G. Cameron and M.M. Pintar 152 (1991) 337
Symmetry breaking in thermally activated NH_4 rotation studied by NMR level crossing spectroscopy, S. Clough, A.J. Horsewill, M.R. Johnson, M.A. Mohammed and T. Newton 152 (1991) 343
Electron relaxation dynamics of Mu ALCR spectra, S.R. Kreitzman 152 (1991) 353
Fluorescence detected level-anticrossing and spin coherence of a localized triplet state in diamond, E. van Oort and M. Glasbeek 152 (1991) 365
Electron spin exchange in micellized radical pairs. I. ^{13}C low field chemically induced dynamic nuclear polarization (CIDNP) and ^{13}C radio frequency stimulated nuclear polarization (SNP), I.A. Shkrob, V.F. Tarasov and E.G. Bagryanskaya 153 (1991) 427
Electron spin exchange in micellized radical pairs. II. Magnetic field and magnetic isotope effects in multinuclear pairs, I.A. Shkrob, V.F. Tarasov and A.L. Buchachenko 153 (1991) 443
Structure of MQ-NMR spin spaces under higher $\mathcal{S}_n$- and $(\mathcal{S}_n)_{\downarrow}\mathcal{G}$ symmetries. II. $\Gamma/\tilde{\Gamma}$ $(\mathcal{S}_6)_{\downarrow}\mathcal{O}$ subduced irreps for sixfold spin clusters pertaining to the molecular cage ion, $[^{11}BH]_6^{2-}$, J.P. Colpa and F.P. Temme 154 (1991) 97
Structure of MQ-NMR spin spaces under higher $\mathcal{S}_n$- and $(\mathcal{S}_n)_{\downarrow}\mathcal{G}$ symmetries. III. $\Gamma/\tilde{\Gamma}$ $((\mathcal{S}_7)_{\downarrow}D_5)$ subduced irreps for $[A]_7$ clusters pertaining to the molecular cage ion, $[^{11}BH]_7^{2-}$, F.P. Temme and J.P. Colpa 154 (1991) 111
^{14}N NQR investigation of some thermochromic and photochromic salicylideneanilines and related compounds, E. Hadjoudis, F. Milia, J. Seliger, V. Zagar and R. Blinc 156 (1991) 149
Intramolecular dynamics of the C_4H_8NH radical cation. An application of the anisotropic exchange theory for powder ESR lineshapes, L. Sjöqvist, N.P. Benetis, A. Lund and J. Maruani 156 (1991) 457

Structure of MQ-NMR spin spaces under higher $\mathscr{S}_n$- and $(\mathscr{S}_n)_\downarrow \mathscr{G}$ symmetries. II. $\Gamma/\tilde{\Gamma}$ $(\mathscr{S}_6)_\downarrow \mathscr{O}$ subduced irreps for sixfold spin clusters pertaining to the molecular cage ion, $[^{11}BH]_6^{2-}$, Chem. Phys. 154 (1991) 97–110. Erratum, J.P. Colpa and F.P. Temme 156 (1991) 532
Optically detected magnetic resonance study of the phosphorescent states of trans-2,2′-bipyridine, metal-free cis-2,2′-bipyridine and $[Zn(bpy)]^{2+}$, M. Yagi, B.D. Schlyer and A.H. Maki 157 (1991) 209
Spinning-rate depedence of ^{31}P magic-angle-spinning nuclear magnetic resonance spectra in condensed phosphates, S. Hayashi and K. Hayamizu 157 (1991) 381
Pulsed field gradient NMR for the study of the structure of membrane systems, V.A. Daragan and E.E. Ilyina 158 (1991) 105
An NMR study of the backbone dynamics of staphylococcal nuclease in the crystalline state, H.B.R. Cole and D.A. Torchia 158 (1991) 271
Hydrogen-exchange labeling study of the allosteric R-state to T-state equilibrium in methemoglobin, R.E. McKinnie, J.J. Englander and S.W. Englander 158 (1991) 283
^{23}Na relaxation in DNA solutions. Influence of intercalation on correlation times and coupling constants, M. Hald and J.P. Jacobsen 159 (1992) 257
Optical and ODMR spectroscopy of an induced triplet X-trap in 1,4-dibromobenzene single crystals, B. Stein, F. Rothamel, T. Kirski, J. Kolenda and C. von Borczyskowski 159 (1992) 269
Methyl tunnelling in solid diacetyl, A.M. Alsanoosi and A.J. Horsewill 160 (1992) 25
Theory of geminate recombination of radical pairs with instantaneously changing spin Hamiltonian. I. General theory and kinematic approximation, A.B. Doktorov, S.A. Mikhailov and P.A. Purtov 160 (1992) 223
Theory of geminate recombination of radical pairs with instantaneously changing spin-Hamiltonian. II. Method of summation of re-encounter contributions, A.B. Doktorov, S.A. Mikhailov and P.A. Purtov 160 (1992) 239
Single-crystal EPR and ^{15}N powder ENDOR studies of $[(C_4H_9)_4N][Tc^{VI}NBr_4/Tc^{V}OBr_4]$, K. Köhler, R. Kirmse, R. Böttcher and U. Abram 160 (1992) 281
The structure and dynamics of 1,3,5-cycloheptatriene and 1,3-cycloheptadiene radical cations in low temperature matrices. An ESR investigation, Y. Kubozono, T. Miyamoto, M. Aoyagi, M. Ata, Y. Matsuda, Y. Gondo, H. Nakamura and T. Matsuo 160 (1992) 421

Microwave spectroscopy

The submillimeter rotation-tunneling spectrum of $Ar–D_2O$ and $Ar–NH_3$, E. Zwart and W.L. Meerts 151 (1991) 407
Observation of level crossing and level anticrossing signals in the CO_2 laser Stark spectrum of POF_3 and their proposed application to electric field standards in laser Stark spectroscopy, K. Tanaka, K. Someya and T. Tanaka 152 (1991) 229
The diagmagnetic properties of the $\cdot NF_2$ radical by magic doublet rotational Zeeman spectroscopy, U.E. Frank and W. Hüttner 152 (1991) 261
The magnetizability and *g*-factor surfaces of ammonia, S.P.A. Sauer, V. Špirko and J. Oddershede 153 (1991) 189
Rotational spectrum and structure of the linear HCN–HCCH dimer, A.I. Jaman, T.C. Germann, H.S. Gutowsky, J.D. Augspurger and C.E. Dykstra 154 (1991) 281
Vibrational energy transfer in the N_2^*–OCS system. Measurements of vibrational populations of the bending manifold in the perturbed steady state by microwave spectroscopy, L.B. Favero, M.C. Righetti and P.G. Favero 155 (1991) 107
Optothermal-detected microwave-sideband CO_2-laser spectroscopy of $NCH–NH_3$, G.T. Fraser, A.S. Pine, W.A. Kreiner and R.D. Suenram 156 (1991) 523

Infrared spectroscopy
The submillimeter rotation-tunneling spectrum of Ar–D_2O and Ar–NH_3, E. Zwart and W.L. Meerts 151 (1991) 407
FIR LMR spectra of FO_2: some classic examples of level anticrossing resonances, U. Bley, P.B. Davies, M. Grantz, T.J. Sears and F. Temps 152 (1991) 281
Proton transfer dynamics in the hydrogen bond. Inelastic neutron scattering, infrared and Raman spectra of $Na_3H(SO_4)_2$, $K_3H(SO_4)_2$ and $Rb_3H(SO_4)_2$, F. Fillaux, A. Lautié, J. Tomkinson and G.J. Kearley 154 (1991) 135
Circular birefringence and dichroism due to shear stress: optical measurement of non-Newtonian viscosity, M.W. Evans 154 (1991) 193
Triplet state IR spectroscopy of aromatic homocycles and heterocycles, H. Krumschmidt and C. Kryschi 154 (1991) 459
The vibrational spectra of the monohalogenated cyclopropanes: ab initio calculations and an experimental study of fluorocyclopropane, C. Kaupert, H. Heydtmann and W. Thiel 156 (1991) 85
Laser-initiated chain reactions and microexplosions in solid solutions of methylcyclopropane and chlorine, T.J. Tague Jr. and C.A. Wight 156 (1991) 141
Optothermal-detected microwave-sideband CO_2-laser spectroscopy of NCH–NH_3, G.T. Fraser, A.S. Pine, W.A. Kreiner and R.D. Suenram 156 (1991) 523
Ring-puckering and internal rotation barriers in N,N′-dimethylethyleneurea, J.C. Otero, J.I. Marcos, E. López-Cantarero and A. Chacón 157 (1991) 201
Laser-initiated chain reactions and microexplosions in solid solutions of methylcyclopropane and chlorine, Chem. Phys. 156 (1991) 141–148. Erratum, T.J. Tague Jr. and C.A. Wright 157 (1991) 305
Proton-transfer dynamics in the hydrogen bond. Inelastic neutron scattering, infrared and Raman spectra of $KH(CF_3COO)_2$ and $CsH(CF_3COO)_2$, F. Fillaux and J. Tomkinson 158 (1991) 113
Time- and temperature dependence of large-scale conformational transitions in myoglobin, R.D. Young, H. Frauenfelder, J.B. Johnson, D.C. Lamb, G.U. Nienhaus, R. Philipp and R. Scholl 158 (1991) 315
Determination of Fe–CO geometry and heme rigidity in carbonmonoxyhemoglobin using femtosecond IR spectroscopy, B. Locke, T. Lian and R.M. Hochstrasser 158 (1991) 409
Collision-induced emission of $O_2(a^1\Delta_g \rightarrow X^3\Sigma_g^-)$ in the gas phase, J. Wildt, E.H. Fink, P. Biggs, R.P. Wayne and A.F. Vilesov 159 (1992) 127
A matrix isolation study of the water–formaldehyde complex. The far-infrared region, B. Nelander 159 (1992) 281
Structural and spectral consequences of ion-pairing. VI. $BO_2^-Li^+$ and $BO_2^-Na^+$, J.S. Francisco and I.H. Williams 160 (1992) 255
Sub-picosecond time-resolved IR spectroscopy of the vibrational dynamics of $Rh(CO)_2(acac)$, J.D. Beckerle, M. Casassa, R.R. Cavanagh, E.J. Heilweil and J.C. Stephenson 160 (1992) 487

Raman spectroscopy
Polar phonons in SO_2 single crystal, A. Tafi, P. Procacci, E. Castellucci and P.R. Salvi 151 (1991) 205
Frequency-dependent solvent friction and torsional damping in liquid 1,2-difluoroethane, R.A. MacPhail and F.C. Monroe 152 (1991) 93
Proton transfer dynamics in the hydrogen bond. Inelastic neutron scattering, infrared and Raman spectra of $Na_3H(SO_4)_2$, $K_3H(SO_4)_2$ and $Rb_3H(SO_4)_2$, F. Fillaux, A. Lautié, J. Tomkinson and G.J. Kearley 154 (1991) 135
Methyl torsion in $C_2H_{4-n}(CH_3)_n$, $n=1$ or 2, R. Engeln and J. Reuss 156 (1991) 215

Ring-puckering and internal rotation barriers in N,N′-dimethylethyleneurea, J.C. Otero, J.I. Marcos, E. López-Cantarero and A. Chacón 157 (1991) 201
Proton-transfer dynamics in the hydrogen bond. Inelastic neutron scattering, infrared and Raman spectra of $KH(CF_3COO)_2$ and $CsH(CF_3COO)_2$, F. Fillaux and J. Tomkinson 158 (1991) 113
Evidence for proximal control of ligand specificity in hemeproteins: absorption and Raman studies of cryogenically trapped photoproducts of ligand bound myoglobins, A.M. Ahmed, B.F. Campbell, D. Caruso, M.R. Chance, M.D. Chavez, S.H. Courtney, J.M. Friedman, I.E.T. Iben, M.R. Ondrias and M. Yang 158 (1991) 329
Electronic spectra of the naphthyridines: 2,7-naphthyridine, P. Wormell and A.R. Lacey 160 (1992) 55
Structural and spectral consequences of ion-pairing. VI. $BO_2^-Li^+$ and $BO_2^-Na^+$, J.S. Francisco and I.H. Williams 160 (1992) 255
Evidence for a gauche minor-conformer of 1,3-butadiene, R. Engeln, D. Consalvo and J. Reuss 160 (1992) 427

Visible and UV spectroscopy

The electronically excited states of 2-phenylindole, B. Albinsson, S. Eriksson, R. Lyng and M. Kubista 151 (1991) 149
Spectroscopy and relaxation dynamics of metastable electronically excited states of iodine in rare gas matrices, M. Macler and M.C. Heaven 151 (1991) 219
Quenching and rotational transfer rates in the $v'=0$ manifold of $OH(A^2\Sigma^+)$, J. Burris, J. Butler, T. McGee and W. Heaps 151 (1991) 233
Excitation and ionization of freon molecules. II. Absolute oscillator strengths for the photoabsorption (7.5–200 eV) and the ionic photofragmentation (12.5–80 eV) of CF_3Cl, W. Zhang, G. Cooper, T. Ibuki and C.E. Brion 151 (1991) 343
Excitation and ionization of freon molecules. III. Absolute oscillator strengths for the photoabsorption (8.5–200 eV) and the ionic photofragmentation (11.5–70 eV) of CF_2Cl_2, W. Zhang, G. Cooper, T. Ibuki and C.E. Brion 151 (1991) 357
A study of the $S_1\ 6^1(^1A_2'')$ vibronically excited state of sym-triazine by high-resolution UV laser spectroscopy, P. Uijt de Haag, W.L. Meerts and J.T. Hougen 151 (1991) 371
Picosecond Stokes shift studies of solvent friction: experimental measurements of time-dependent band shape and integrated intensity, J.D. Simon and S.-G. Su 152 (1991) 143
Anomalous behavior of the anticrossing density as a function of excitation energy in the C_2H_2 molecule, P. Dupré, R. Jost, M. Lombardi, P.G. Green, E. Abramson and R.W. Field 152 (1991) 293
Rovibronic level structure of electronically excited acetylene ($\tilde{A}\,^1A_u$) in a supersonic jet as studied by laser-induced fluorescence and Zeeman quantum beat spectroscopy, N. Ochi and S. Tsuchiya 152 (1991) 319
Mixing of the vibrational angular momentum components of multiply degenerate vibronic states of benzene by vibrational *l*-type resonance, E. Riedle and J. Pliva 152 (1991) 375
The influence of the spin–orbit and the hyperfine interaction on the asymptotic behaviour of the $A\,^1\Sigma_u^+$ state of Na_2, H. Knöckel, T. Johr, H. Richter and E. Tiemann 152 (1991) 399
Dissociative excitation of hydrogen in rf and dc glow discharges through H_2, S.B. Vrhovac, S.B. Radovanov, S.A. Bzenić, Z.Lj. Petrović and B.M. Jelenković 153 (1991) 233
Excitation and ionization of freon molecules. IV. Absolute oscillator strengths for the photoabsorption (6–200 eV) and the ionic photofragmentation (11.5–49 eV) of $CFCl_3$, W. Zhang, G. Cooper, T. Ibuki and C.E. Brion 153 (1991) 491
Multiphoton dissociation dynamics of highly excited states of CS_2 and CS_2 clusters, E. Patsilinakou, D. Proch and C. Fotakis 153 (1991) 503

Resonant two-photon ionization of phenol in methylene chloride doped solid argon using 248 nm KrF laser and 254 nm Hg lamp radiation, a comparative study. The UV/VIS absorption spectrum of phenol radical cation, K. Kesper, F. Diehl, J.G.G. Simon, H. Specht and A. Schweig 153 (1991) 511

The $C(^3P_J)+NO(X^2\Pi_r)\rightarrow CN(X^2\Sigma^+)+O(^3P_J)$ reaction dynamics studied at 0.06 and 0.23 eV relative translational energy in pulsed crossed supersonic molecular beams, C. Naulin, M. Costes and G. Dorthe 153 (1991) 519

Emission of $Xe:N(^2P)$ collision complexes near the $N(^2P\rightarrow{}^2D)$ lines, A.F. Vilesov, J. Wildt and E.H. Fink 153 (1991) 531

Anomalous behaviour of the anticrossing density as a function of excitation energy in the C_2H_2 molecule, Chem. Phys. 152 (1991) 293. Erratum, P. Dupré, R. Jost, M. Lombardi, P.G. Green, E. Abramson and R.W. Field 153 (1991) 539

Model calculations of the anthracene photocurrent spectrum, P. Petelenz and D. Mucha 154 (1991) 145

Photochromic thiophenefulgides. Photokinetics of two isopropyl derivatives, K. Ulrich, H. Port, H.C. Wolf, J. Wonner, F. Effenberger and H.-D. Ilge 154 (1991) 311

Energy levels of Cr^{3+} ions in C_{3i} sites of $Y_3Al_5O_{12}$, C.A. Morrison, J.B. Gruber and M.E. Hills 154 (1991) 437

High pressure study of intermolecular resonance interaction in a naphthalene crystal, K.P. Meletov 154 (1991) 469

The optical spectrum of $Ba_2Zn[Cu]F_6$, D. Reinen, G. Steffen, M.A. Hitchman, H. Stratemeier, L. Dubicki, E.R. Krausz, M.J. Riley, H.E. Mathies, K. Recker and F. Wallrafen 155 (1991) 117

Laser excitation and resolved emission spectra of supersonically cooled aluminum dimer, M.F. Cai, C.C. Carter, T.A. Miller and V.E. Bondybey 155 (1991) 233

A cluster model of the charge transfer interaction between an impurity and the host molecular crystal, P. Petelenz and A. Eilmes 155 (1991) 247

Photoionisation and ZEKE photoelectron spectroscopy of Ar, H_2 and CO_2 using a coherent XUV laser source, H.H. Fielding, T.P. Softley and F. Merkt 155 (1991) 257

On the BiF bond dissociation energy and an evaluation of the BiF red emission band systems, T.C. Devore, L. Brock, R. Kahlscheuer, K. Dulaney and J.L. Gole 155 (1991) 423

Circular dichroism spectrum of gadolinium diglycolate single crystal, T. Kundu, A.K. Banerjee and M. Chowdhury 156 (1991) 95

Electronic spectra of 4-nitro-pyridine-*n*-oxide (NPO) single crystals, M. Pierre, P.L. Baldeck, D. Block, R. Georges, H.P. Trommsdorff and J. Zyss 156 (1991) 103

Pressure dependence of the polarized reflectance spectrum of a solid charge-transfer complex, perylene-hexacyanobutadiene (HCBD), T. Ida, K. Yakushi, H. Kuroda, H. Yamochi and G. Saito 156 (1991) 113

On the BiF bond dissociation energy and an evaluation of the BiF red emission band systems, Chem. Phys. 155 (1991) 423–433. Erratum, T. Devore, L. Brock, R. Kahlscheuer, K. Dulaney and J.L. Gole 156 (1991) 156

Vibrational and rotational effects on the intersystem crossing in pyrazine and pyrimidine, P. Uijt de Haag and W.L. Meerts 156 (1991) 197

Magnetic field dependence of rotationally resolved excitation spectra of the $^1B_{3u}$ 0_0^0 transition of jet-cooled pyrazine, P.J. de Lange, H.Th. Jonkman and K.E. Drabe 156 (1991) 209

The trans-stilbene–Ar van der Waals complex. Vibrationally averaged substitution structure in its S_0 and S_1 electronic states, B.B. Champagne, D.F. Plusquellic, J.F. Pfanstiel, D.W. Pratt, W.M. van Herpen and W.L. Meerts 156 (1991) 251

Electronic spectra and proton transfer in the phenol/$(NH_3)_n$ clusters in argon matrices, C. Crépin and A. Tramer 156 (1991) 281
Two-dimensional model of charge transfer excitons in polyacene crystals, P. Petelenz and M. Slawik 157 (1991) 169
The potential of the Na_2 $B^1\Pi_u$ state, H. Richter, H. Knöckel and E. Tiemann 157 (1991) 217
Pressure dependence of the polarized reflectance spectrum of a solid charge-transfer complex, perylene-hexacyanobutadiene (HCBD), Chem. Phys. 156 (1991) 113–122. Erratum, T. Ida, K. Yakushi, H. Kuroda, H. Yamochi and G. Saito 157 (1991) 305
Absorption spectra of a solvated electron in ethers, H. Abramczyk and J. Kroh 157 (1991) 373
Diffusion of molecular oxygen in pairs (anthracene–O_2) in glassy matrices, V.V. Korolev, D.G. Sushkov and N.M. Bazhin 158 (1991) 129
Charged substituents and the effect of their electric field on the electronic spectra of some aminocoumarins, S.I. Druzhinin, B.D. Bursulaya and B.M. Uzhinov 158 (1991) 137
Protein relaxation dynamics in human myoglobin, D.G. Lambright, S. Balasubramanian and S.G. Boxer 158 (1991) 249
Time- and temperature dependence of large-scale conformational transitions in myoglobin, R.D. Young, H. Frauenfelder, J.B. Johnson, D.C. Lamb, G.U. Nienhaus, R. Philipp and R. Scholl 158 (1991) 315
Evidence for proximal control of ligand specificity in hemeproteins: absorption and Raman studies of cryogenically trapped photoproducts of ligand bound myoglobins, A.M. Ahmed, B.F. Campbell, D. Caruso, M.R. Chance, M.D. Chavez, S.H. Courtney, J.M. Friedman, I.E.T. Iben, M.R. Ondrias and M. Yang 158 (1991) 329
Collision-induced emission of $O_2(a^1\Delta_g \rightarrow X^3\Sigma_g^-)$ in the gas phase, J. Wildt, E.H. Fink, P. Biggs, R.P. Wayne and A.F. Vilesov 159 (1992) 127
Ab initio study of the vibrational structure of the X^2A_1 and A^2B_1 electronic states of CH_2^+, W. Reuter and S.D. Peyerimhoff 160 (1992) 11
Electronic spectra of the naphthyridines: 2,7-naphthyridine, P. Wormell and A.R. Lacey 160 (1992) 55
CuBr chemiluminescence from the $Cu^*(^2D_{3/2,5/2}) + Br_2$ reaction, P. Kowalczyk, I. Hikmet and N. Sadeghi 160 (1992) 73
On the photo-sensitized injection of electrons into SnO_2 from cyanine dyes incorporated in Langmuir–Blodgett films, G. Biesmans, M. Van der Auweraer, C. Cathry, F.C. De Schryver, Y. Yonezawa and T. Sato 160 (1992) 97
On the mechanism of radiationless deactivation of rhodamines, T. López Arbeloa, F. López Arbeloa, P.H. Bartolomé and I. López Arbeloa 160 (1992) 123
Absolute dipole differential oscillator strengths for inner shell spectra from high resolution electron energy loss studies of the freon molecules CF_4, CF_3Cl, CF_2Cl_2, $CFCl_3$ and CCl_4, W. Zhang, T. Ibuki and C.E. Brion 160 (1992) 435
Electronic spectra and transitions of the fullerene C_{60}, S. Leach, M. Vervloet, A. Desprès, E. Bréheret, J.P. Hare, T.J. Dennis, H.W. Kroto, R. Taylor and D.R.M. Walton 160 (1992) 451

Fluorescence spectroscopy

The electronically excited states of 2-phenylindole, B. Albinsson, S. Eriksson, R. Lyng and M. Kubista 151 (1991) 149
Spectroscopy and relaxation dynamics of metastable electronically excited states of iodine in rare gas matrices, M. Macler and M.C. Heaven 151 (1991) 219
Quenching and rotational transfer rates in the $v' = 0$ manifold of $OH(A^2\Sigma^+)$, J. Burris, J. Butler, T. McGee and W. Heaps 151 (1991) 233

Picosecond photodissociation and geminate radical recombination in alkane solutions of tetraphenylhydrazine, M.G. Hyde and G.S. Beddard 151 (1991) 239
Photoisomerization dynamics of diphenylbutadiene in compressed liquid alkanes and in solid environment, Ch. Gehrke, R. Mohrschladt, J. Schroeder, J. Troe and P. Vöhringer 152 (1991) 45
Friction effect on the mechanism of photochemical redox processes in solutions, E.I. Kapinus 152 (1991) 83
Picosecond Stokes shift studies of solvent friction: experimental measurements of time-dependent band shape and integrated intensity, J.D. Simon and S.-G. Su 152 (1991) 143
Fluorescence detected level-anticrossing and spin coherence of a localized triplet state in diamond, E. van Oort and M. Glasbeek 152 (1991) 365
Near- and non-resonant (VV) energy transfer between molecules dissolved in liquid krypton: a comparison with liquid argon, J.J. Andrew, D.C. McDermott, S.P. Mills and C.J.S.M. Simpson 153 (1991) 247
The $C(^3P_J)+NO(X^2\Pi_r)\rightarrow CN(X^2\Sigma^+)+O(^3P_J)$ reaction dynamics studied at 0.06 and 0.23 eV relative translational energy in pulsed crossed supersonic molecular beams, C. Naulin, M. Costes and G. Dorthe 153 (1991) 519
A femtosecond study of electronic state dynamics of fucoxanthin and implications for photosynthetic carotenoid-to-chlorophyll energy transfer mechanisms, A.P. Shreve, J.K. Trautman, T.G. Owens and A.C. Albrecht 154 (1991) 171
Excimer geometries in bichromophoric molecules: a theoretical and experimental study of 1,2-(bis-9-antrhyl)-ethane, G.D. Scholes, K.P. Ghiggino and G.J. Wilson 155 (1991) 127
Dissociative excitation of SiH_4 by electron impact: emission cross sections for the hydrogen Lyman series, S. Tsurubuchi, K. Motohashi, S. Matsuoka and T. Arikawa 155 (1991) 401
A fluorescence characterization of the *p*-difluorobenzene–argon van der Waals complex. Energy levels, geometries and dissociation energies, M.-C. Su, H.-K. O and C.S. Parmenter 156 (1991) 261
Electronic spectra and proton transfer in the phenol/$(NH_3)_n$ clusters in argon matrices, C. Crépin and A. Tramer 156 (1991) 281
Fluorescence analysis of two new TICT systems: 10-cyano-9,9′-bianthryl (CBA) and 10,10′-dicyano-9,9′-bianthryl (DCBA), S. Müller and J. Heinze 157 (1991) 231
Singlet excitation energy transfer in tetracene doped *p*-terphenyl single crystals, A. Krüger, C. Kryschi, L. Valkunas and D. Schmid 157 (1991) 243
A time-resolved fluorescence study of electronic excitation energy transport in concentrated dye solutions, A.D. Scully, A. Matsumoto and S. Hirayama 157 (1991) 253
On the fluorescence depolarization in bis-(N-carbazolyl) compounds, M. Hennecke and H.F. Kauffmann 157 (1991) 391
Radiative lifetimes of confined excitations in sigma-conjugated silane oligomers, J.R.G. Thorne, S.A. Williams, R.M. Hochstrasser and P.J. Fagan 157 (1991) 401
Diffusion of molecular oxygen in pairs (anthracene–O_2) in glassy matrices, V.V. Korolev, D.G. Sushkov and N.M. Bazhin 158 (1991) 129
Charged substituents and the effect of their electric field on the electronic spectra of some aminocoumarins, S.I. Druzhinin, B.D. Bursulaya and B.M. Uzhinov 158 (1991) 137
Radiative and radiationless depopulation of the excited intramolecular charge transfer states: aryl derivatives of aromatic amines, J. Herbich and A. Kapturkiewicz 158 (1991) 143
Site-resolved vibronic spectra of matrix-isolated NBr: comparison with model calculations, K. Seranski, M. Winter and U. Schurath 159 (1992) 247
Optical and ODMR spectroscopy of an induced triplet X-trap in 1,4-dibromobenzene single crystals, B. Stein, F. Rothamel, T. Kirski, J. Kolenda and C. von Borczyskowski 159 (1992) 269

Fluorescence excitation spectrum of 1,8-disubstituted naphthalenes in supersonic jet, T. Chakraborty and M. Chowdhury 159 (1992) 439
Theoretical and experimental study on the electronic spectrum and photophysics of Michler's hydrol blue, I. Baraldi, A. Carnevali, F. Momicchioli and G. Ponterini 160 (1992) 85
Principal-component self-modeling analysis of fluorescence for some trans-diarylethylenes. A comparison with kinetic analysis, A. Spalletti, G. Bartocci, F. Masetti, U. Mazzucato and G. Cruciani 160 (1992) 131
Temperature dependence of the fluorescence spectra of poly-N-vinylcarbazole films from 300 to 550 K: evidence for monomer emission, G. Giro and G. Orlandi 160 (1992) 145
Intramolecular charge transfer and trans–cis isomerization of the DCM styrene dye in polar solvents. A CS INDO MRCI study, S. Marguet, J.C. Mialocq, P. Millie, G. Berthier and F. Momicchioli 160 (1992) 265

Photoelectron and Auger spectroscopy
Core excitation-induced photodesorption of molecular and fragment ions from CO adsorbates on metal surfaces, R. Treichler, W. Wurth, W. Riedl, P. Feulner and D. Menzel 153 (1991) 259
Unusual features in the polarised single crystal electronic spectrum of $(NH_4)_2[V(H_2O)_6](SO_4)_2$: analysis of Fano antiresonance structure and bonding in the $[V(H_2O)_6]^{2+}$ complex, R.G. McDonald, R. Stranger, M.A. Hitchman and P.W. Smith 154 (1991) 179
Model potentials in numerical local density functional methods, G.L. Gutsev, V.K. Gryaznov and V.A. Nasluzov 154 (1991) 291
Absolute partial photoionization cross sections of ethylene, F.A. Grimm, T.A. Whitley, P.R. Keller and J.W. Taylor 154 (1991) 303
Photoionisation and ZEKE photoelectron spectroscopy of Ar, H_2 and CO_2 using a coherent XUV laser source, H.H. Fielding, T.P. Softley and F. Merkt 155 (1991) 257
Experimental and theoretical study of the N_{1s} and C_{1s} shake-up satellites in pyridine and aniline, M.P. Keane, A. Naves de Brito, N. Correia, S. Svensson and S. Lunell 155 (1991) 379
The treatment of electron correlation in aperiodic systems. IV. Exciton bands and double ionization potentials, C.-M. Liegener 157 (1991) 183
The electronic states of the azines. V. Pyridazine, studied by VUV absorption, near threshold electron energy-loss spectroscopy and ab initio multi-reference configuration interaction calculations, M.H. Palmer and I.C. Walker 157 (1991) 187
UV photoemission spectroscopic studies on molecular aggregation of triphenylamines dispersed in polycarbonate thin films, N. Sato and M. Yoshikawa 160 (1992) 289
The electronic structure of poly(*p*-phenylene vinylene), N. Sato, M. Lögdlund, R. Lazzaroni, W.R. Salaneck, J.-L. Brédas, D.D.C. Bradley, R.H. Friend and K.E. Ziemelis 160 (1992) 299

X-ray spectroscopy
Oxygen K-shell excitation spectroscopy of hydrogen peroxide, E. Rühl and A.P. Hitchcock 154 (1991) 323
Shape resonances in low-energy electron transmission and sulfur K-shell photoabsorption spectroscopies: CH_3SH, C_2H_5SH, $(CH_3)_2S$, $(C_2H_5)_2S$, C_6H_5SH, $C_6H_5SCH_3$, CH_3SCN, CH_3NCS, SCl_2, C. Dezarnaud, M. Tronc and A. Modelli 156 (1991) 129

Electron impact spectroscopy
Jahn–Teller effect and dissociation from the ground state of CF_4^+, J.M. García de la Vega and E. San Fabián 151 (1991) 335

The electronic states of the azines. IV. Pyrazine, studied by VUV absorption, near-threshold electron energy-loss spectroscopy and ab initio multi-reference configuration interaction calculations, I.C. Walker and M.H. Palmer 153 (1991) 169
Estimation of the integral cross section for dissociative excitation of F_2 by electron impact, D.C. Cartwright, P.J. Hay and S. Trajmar 153 (1991) 219
Production of the N_2 ($A^3\Sigma_u^+$) metastable state by electron impact dissociative excitation of N_2O, S.M. Barnett, N.J. Mason and W.R. Newell 153 (1991) 283
Oxygen K-shell excitation spectroscopy of hydrogen peroxide, E. Rühl and A.P. Hitchcock 154 (1991) 323
Lowest energy triplet states of group Vb hydrides: NH_3 (ND_3) and PH_3, M. Ben Arfa and M. Tronc 155 (1991) 143
Valence-shell electron momentum distributions of cyclopropane by symmetric noncoplanar (e,2e) spectroscopy, M.P. Banjavčić, T.A. Daniels and K.T. Leung 155 (1991) 309
Shape resonances in low-energy electron transmission and sulfur K-shell photoabsorption spectroscopies: CH_3SH, C_2H_5SH, $(CH_3)_2S$, $(C_2H_5)_2S$, C_6H_5SH, $C_6H_5SCH_3$, CH_3SCN, CH_3NCS, SCl_2, C. Dezarnaud, M. Tronc and A. Modelli 156 (1991) 129
Dissociation of aliphatic hydrocarbons excited by electrons: translational energy distributions of the excited hydrogen atom, T. Ogawa, T. Tsuboi and K. Nakashima 156 (1991) 465
Dissociation of hydrogen sulfide in e–H_2S collisions: translational energy distribution of $H^*(n=4)$, T. Ogawa, M. Tsukada and K. Nakashima 156 (1991) 473
Rotational distributions of $N_2O^+(\tilde{A}^2\Sigma^+)$, $CO_2^+(\tilde{A}^2\Pi_u)$ and $CS_2^+(\tilde{A}^2\Pi_u)$ produced by electron-impact ionization, I. Tokue, A. Masuda, H. Kume and Y. Ito 158 (1991) 161
Valence-shell electron momentum distributions and ionization energy spectra of tetramethylsilane by symmetric noncoplanar (e, 2e) spectroscopy, T. Daniels, H. Zhu, M.P. Banjavčić and K.T. Leung 159 (1992) 289
Assessment of Gaussian-weighted angular resolution functions in the comparison of quantum-mechanically calculated electron momentum distributions with experiment, P. Duffy, M.E. Casida, C.E. Brion and D.P. Chong 159 (1992) 347
Absolute dipole differential oscillator strengths for inner shell spectra from high resolution electron energy loss studies of the freon molecules CF_4, CF_3Cl, CF_2Cl_2, $CFCl_3$ and CCl_4, W. Zhang, T. Ibuki and C.E. Brion 160 (1992) 435

Laser methods

Determination of the radiative lifetimes of nine ion-pair states of I_2, P.J. Jewsbury, K.P. Lawley, T. Ridley, F.F. Al-Adel, P.R.R. Langridge-Smith and R.J. Donovan 151 (1991) 103
Secondary heating effects in laser-induced fluorescence experiments, K.L. McNesby and R.D. Bates Jr. 151 (1991) 385
CO_2 laser-induced fluorescence studies of vibrational energy transfer in N_2O, K.L. McNesby and R.D. Bates Jr. 151 (1991) 401
Observation of level crossing and level anticrossing signals in the CO_2 laser Stark spectrum of POF_3 and their proposed application to electric field standards in laser Stark spectroscopy, K. Tanaka, K. Someya and T. Tanaka 152 (1991) 229
FIR LMR spectra of FO_2: some classic examples of level anticrossing resonances, U. Bley, P.B. Davies, M. Grantz, T.J. Sears and F. Temps 152 (1991) 281
Anomalous structure in the $A^6\Sigma^+$–$X^6\Sigma^+$ transition of MnO caused by interference between two internal hyperfine perturbations, A.G. Adam, Y. Azuma, H. Li, A.J. Merer and C. Thambir 152 (1991) 391

Highly excited states of nitric oxide studied by high-resolution resonance-enhanced multiphoton ionization spectroscopy, Y. Luo, Y.D. Cheng, H. Ågren, R. Maripuu, W. Seibt, L. Öhlund, P. Ejeklint, B. Carman, K.Z. Xing, Y. Achiba and K. Siegbahn 153 (1991) 473
Kinetics and magnetic field effect in geminate recombination of triplet radical pairs adsorbed onto porous glass studied by laser flash technique, P.P. Levin, I.V. Katalnikov and V.A. Kuzmin 154 (1991) 449
Photoionisation and ZEKE photoelectron spectroscopy of Ar, H_2 and CO_2 using a coherent XUV laser source, H.H. Fielding, T.P. Softley and F. Merkt 155 (1991) 257
Pulsed discharge source of supersonically cooled transient species, R. Schlachta, G. Lask, S.H. Tsay and V.E. Bondybey 155 (1991) 267
Photodissociation of CF_3I at 248 nm: kinetic energy dependence of the recoil anisotropy, P. Felder 155 (1991) 435
Laser-initiated chain reactions and microexplosions in solid solutions of methylcyclopropane and chlorine, T.J. Tague Jr. and C.A. Wight 156 (1991) 141
S_1–T_1 coupling in propynal by level anticrossing spectroscopy, M. Lombardi, J.P. Pique, U. Brühlmann and J.R. Huber 156 (1991) 163
Isomer-specific radiative lifetimes of molecular heteroclusters, D. Bahatt, U. Even, E. Shalev, N. Ben-Horin and J. Jortner 156 (1991) 223
Real-time dynamics of vibrational predissociation in anthracene–Ar_n ($n=1,2,3$), A. Heikal, L. Bañares, D.H. Semmes and A.H. Zewail 156 (1991) 231
State-to-state cross sections for rotational excitation of ortho- and para-NH_3 by He and H_2, J. Schleipen and J.J. ter Meulen 156 (1991) 479
Laser excitation of the $A\,^3\Sigma_u^+$, $A'\,^3\Delta_u$ and $c\,^1\Sigma_u^-$ states of molecular oxygen, J. Wildt, G. Bednarek, E.H. Fink and R.P. Wayne 156 (1991) 497
The potential of the Na_2 $B\,^1\Pi_u$ state, H. Richter, H. Knöckel and E. Tiemann 157 (1991) 217
Laser-initiated chain reactions and microexplosions in solid solutions of methylcyclopropane and chlorine, Chem. Phys. 156 (1991) 141–148. Erratum, T.J. Tague Jr. and C.A. Wright 157 (1991) 305
Photothermal grating spectroscopy study of nongeminate atom recombination of photodissociated iodine in liquids, X.R. Zhu and J.M. Harris 157 (1991) 409
Intramultiplet relaxation of $Cd(5\,^3P_2)$ induced by collisions with N_2 and CO, A. Masaki, T. Ohnuma, K. Kuwahara, H. Umemoto, Y. Wada, F. Misaizu and K. Fuke 158 (1991) 155
Fluorescence excitation spectrum of 1,8-disubstituted naphthalenes in supersonic jet, T. Chakraborty and M. Chowdhury 159 (1992) 439
CuBr chemiluminescence from the $Cu^*(^2D_{3/2,5/2}) + Br_2$ reaction, P. Kowalczyk, I. Hikmet and N. Sadeghi 160 (1992) 73
Temperature dependence of cyanogen radical reactions with selected alkanes: CN reactivities towards primary, secondary and tertiary C–H bonds, D.L. Yang, T. Yu, N.S. Wang and M.C. Lin 160 (1992) 307
CN radical reactions with selected olefins in the temperature range 174–740 K, D.L. Yang, T. Yu, N.S. Wang and M.C. Lin 160 (1992) 317
Measurement of quadratic hyperpolarizabilities of unsymmetrical donor–acceptor bi- and polyaryls: effect of size and torsion angle of aryl units, G. Puccetti, I. Ledoux, J. Zyss, A. Jutand and C. Amatore 160 (1992) 467

Picosecond spectroscopy

Time-resolved relaxation of one- and two-vibron states in the rubidium perchlorate crystal, G.M. Gale and P. Schanne 151 (1991) 127

Picosecond photodissociation and geminate radical recombination in alkane solutions of tetraphenylhydrazine, M.G. Hyde and G.S. Beddard 151 (1991) 239
Photoisomerization dynamics of diphenylbutadiene in compressed liquid alkanes and in solid environment, Ch. Gehrke, R. Mohrschladt, J. Schroeder, J. Troe and P. Vöhringer 152 (1991) 45
Nonexponential solvation dynamics of simple liquids and mixtures, W. Jarzeba, G.C. Walker, A.E. Johnson and P.F. Barbara 152 (1991) 57
Metal carbonyl photochemistry in organic solvents: femtosecond transient absorption and preliminary resonance Raman spectroscopy, A.G. Joly and K.A. Nelson 152 (1991) 69
Transient spectroscopy of triphenylmethane derivatives following subpicosecond irradiation, M.M. Martin, P. Plaza and Y.H. Meyer 153 (1991) 297
Picosecond time-resolved absorption and fluorescence in the bacteriorhodopsin photocycle: vibrationally-excited species, D. Blanchard, D.A. Gilmore, T.L. Brack, H. Lemaire, D. Hughes and G.H. Atkinson 154 (1991) 155
Vibrational relaxation in crystal SO_2, P. Procacci, A. Tafi, L. Angeloni, R. Righini and P.R. Salvi 154 (1991) 331
Resonant degenerate four wave mixing and scaling laws for saturable absorption in thin films of conjugated polymers and Rhodamine 6G, C. Bubeck, A. Kaltbeitzel, A. Grund and M. LeClerc 154 (1991) 343
Fluorescence depolarization in nonlinear molecular pairs, D. Gülen 156 (1991) 123
Real-time dynamics of vibrational predissociation in anthracene–Ar_n ($n=1,2,3$), A. Heikal, L. Bañares, D.H. Semmes and A.H. Zewail 156 (1991) 231
Radiative lifetimes of confined excitations in sigma-conjugated silane oligomers, J.R.G. Thorne, S.A. Williams, R.M. Hochstrasser and P.J. Fagan 157 (1991) 401
Determination of Fe–CO geometry and heme rigidity in carbonmonoxyhemoglobin using femtosecond IR spectroscopy, B. Locke, T. Lian and R.M. Hochstrasser 158 (1991) 409

Non-linear optical spectroscopy

Time-resolved relaxation of one- and two-vibron states in the rubidium perchlorate crystal, G.M. Gale and P. Schanne 151 (1991) 127
Anomalous structure in the $A^6\Sigma^+$–$X^6\Sigma^+$ transition of MnO caused by interference between two internal hyperfine perturbations, A.G. Adam, Y. Azuma, H. Li, A.J. Merer and C. Thambir 152 (1991) 391
Conformational dependence of the quadratic hyperpolarisabilities of a series of push–pull diaryl acetylenes: an experimental and computational investigation, M. Barzoukas, A. Fort, G. Klein, A. Boeglin, C. Serbutoviez, L. Oswald and J.F. Nicoud 153 (1991) 457
Resonant degenerate four wave mixing and scaling laws for saturable absorption in thin films of conjugated polymers and Rhodamine 6G, C. Bubeck, A. Kaltbeitzel, A. Grund and M. LeClerc 154 (1991) 343
Effects of homogeneous and inhomogeneous broadening mechanisms and molecular rearrangement dynamics on frequency resolved and time resolved coherent Raman intensities, H. Okamoto 155 (1991) 291

Synchrotron spectroscopies

Photoionization mass spectrometry of kinetic energy-selected ions. An ion retarding potential difference method applied to NO^+ and O^+ from N_2O, R. Locht, G. Hagenow, K. Hottmann and H. Baumgärtel 151 (1991) 137

Excitation and ionization of freon molecules. III. Absolute oscillator strengths for the photoabsorption (8.5–200 eV) and the ionic photofragmentation (11.5–70 eV) of CF_2Cl_2, W. Zhang, G. Cooper, T. Ibuki and C.E. Brion 151 (1991) 357
The electronic states of the azines. IV. Pyrazine, studied by VUV absorption, near-threshold electron energy-loss spectroscopy and ab initio multi-reference configuration interaction calculations, I.C. Walker and M.H. Palmer 153 (1991) 169
Core excitation-induced photodesorption of molecular and fragment ions from CO adsorbates on metal surfaces, R. Treichler, W. Wurth, W. Riedl, P. Feulner and D. Menzel 153 (1991) 259
Shape resonances in photoionizations of cyanoacetylene. Experimental and theoretical investigations of the $\tilde{X}\,^2\Pi$, $\tilde{A}\,^2\Sigma$ and $\tilde{B}\,^2\Pi$ ionizations up to a photon energy of 28 eV, J. Kreile, H.-D. Kurland, W. Seibel and A. Schweig 155 (1991) 99
The photoionization of ammonia revisited. The vibrational autoionization of NH_3 and its three isotopomers in the 10–12 eV photon energy range, R. Locht, B. Leyh, W. Denzer, G. Hagenow and H. Baumgärtel 155 (1991) 407
Shape resonances in low-energy electron transmission and sulfur K-shell photoabsorption spectroscopies: CH_3SH, C_2H_5SH, $(CH_3)_2S$, $(C_2H_5)_2S$, C_6H_5SH, $C_6H_5SCH_3$, CH_3SCN, CH_3NCS, SCl_2, C. Dezarnaud, M. Tronc and A. Modelli 156 (1991) 129
The electronic states of the azines. V. Pyridazine, studied by VUV absorption, near threshold electron energy-loss spectroscopy and ab initio multi-reference configuration interaction calculations, M.H. Palmer and I.C. Walker 157 (1991) 187
Core level photoionization mass spectroscopy of the fluoromethylsilanes, $Si(CH_3)_xF_{4-x}$ (x=0–4), around the Si 2p ionization edges, J.D. Bozek, K.H. Tan, G.M. Bancroft and K.J. Fu 158 (1991) 171
Photoionization mass spectrometry of kinetic energy-selected ions. The translational energy distribution of N^+/N_2 in the inner-shell ionization energy range, R. Locht, W. Denzer, E. Rühl and H. Baumgärtel 160 (1992) 477

Coherent optical spectroscopy

Rovibronic level structure of electronically excited acetylene ($\tilde{A}\,^1A_u$) in a supersonic jet as studied by laser-induced fluorescence and Zeeman quantum beat spectroscopy, N. Ochi and S. Tsuchiya 152 (1991) 319

Optical pumping

Total ionization cross sections for Ne**{$(2p)^5(3p)$; J=3}-molecule systems: absolute values and polarization effects, J.P.J. Driessen, M.P.I. Manders, F.J.M. van de Weijer, G.J. Sandker, W. Boom, H.C.W. Beijerinck and B.J. Verhaar 155 (1991) 447
Laser excitation of the $A\,^3\Sigma_u^+$, $A'\,^3\Delta_u$ and $c\,^1\Sigma_u^-$ states of molecular oxygen, J. Wildt, G. Bednarek, E.H. Fink and R.P. Wayne 156 (1991) 497

Multiple resonance spectroscopy

Determination of the radiative lifetimes of nine ion-pair states of I_2, P.J. Jewsbury, K.P. Lawley, T. Ridley, F.F. Al-Adel, P.R.R. Langridge-Smith and R.J. Donovan 151 (1991) 103
Observation of level crossing and level anticrossing signals in the CO_2 laser Stark spectrum of POF_3 and their proposed application to electric field standards in laser Stark spectroscopy, K. Tanaka, K. Someya and T. Tanaka 152 (1991) 229
A Zeeman level crossing study of the symmetry of the potential hindering the torsional oscillator CH_3, W.T. Sobol, I.G. Cameron and M.M. Pintar 152 (1991) 337

Structure of MQ-NMR spin spaces under higher $\mathscr{S}_n$- and $(\mathscr{S}_n)_\downarrow\mathscr{G}$ symmetries. II. $\Gamma/\tilde{\Gamma}$ $(\mathscr{S}_6)_\downarrow\mathscr{O}$ subduced irreps for sixfold spin clusters pertaining to the molecular cage ion, $[^{11}BH]_6^{2-}$, J.P. Colpa and F.P. Temme 154 (1991) 97

Structure of MQ-NMR spin spaces under higher $\mathscr{S}_n$- and $(\mathscr{S}_n)_\downarrow\mathscr{G}$ symmetries. III. $\Gamma/\tilde{\Gamma}$ $((\mathscr{S}_7)_\downarrow D_5)$ subduced irreps for $[A]_7$ clusters pertaining to the molecular cage ion, $[^{11}BH]_7^{2-}$, F.P. Temme and J.P. Colpa 154 (1991) 111

Zeeman effect in the two-photon excitation spectrum of the $C^2\Pi$ state of NO, S. Guizard, N. Shafizadeh, D. Chapoulard, M. Horani and D. Gauyacq 156 (1991) 509

Structure of MQ-NMR spin spaces under higher $\mathscr{S}_n$- and $(\mathscr{S}_n)_\downarrow\mathscr{G}$ symmetries. II. $\Gamma/\tilde{\Gamma}$ $(\mathscr{S}_6)_\downarrow\mathscr{O}$ subduced irreps for sixfold spin clusters pertaining to the molecular cage ion, $[^{11}BH]_6^{2-}$, Chem. Phys. 154 (1991) 97–110. Erratum, J.P. Colpa and F.P. Temme 156 (1991) 532

Single-crystal EPR and ^{15}N powder ENDOR studies of $[(C_4H_9)_4N][Tc^{VI}NBr_4/Tc^{V}OBr_4]$, K. Köhler, R. Kirmse, R. Böttcher and U. Abram 160 (1992) 281

Atomic and molecular beam techniques

A classical study on the vibrational motion of a diatomic molecule in a collisional vibronic excitation, R.F.M. Lobo and A.M.C. Moutinho 151 (1991) 95

Hydroxonium ion formation in collisions of $H_2O^+ + D_2O$ and $D_2O^+ + H_2O$: a crossed-beam scattering study, J. Vančura and Z. Herman 151 (1991) 249

Avoided-crossing molecular-beam study of the torsion–rotation energy levels of CH_3CF_3, W.L. Meerts and I. Ozier 152 (1991) 241

The influence of the spin–orbit and the hyperfine interaction on the asymptotic behaviour of the $A\,^1\Sigma_u^+$ state of Na_2, H. Knöckel, T. Johr, H. Richter and E. Tiemann 152 (1991) 399

An experimental and theoretical study of SF^{q+} $(q=1–3)$ ions, K. Nagesha, V.R. Marathe and D. Mathur 154 (1991) 125

Translational energy study of CH_3 photofragments following $^1(n,\pi^*)$ excitation of acetone, L.D. Waits, R.J. Horwitz and J.A. Guest 155 (1991) 149

On the BiF bond dissociation energy and an evaluation of the BiF red emission band systems, T.C. Devore, L. Brock, R. Kahlscheuer, K. Dulaney and J.L. Gole 155 (1991) 423

Photodissociation of CF_3I at 248 nm: kinetic energy dependence of the recoil anisotropy, P. Felder 155 (1991) 435

Total ionization cross sections for $Ne^{**}\{(2p)^5(3p); J=3\}$-molecule systems: absolute values and polarization effects, J.P.J. Driessen, M.P.I. Manders, F.J.M. van de Weijer, G.J. Sandker, W. Boom, H.C.W. Beijerinck and B.J. Verhaar 155 (1991) 447

On the BiF bond dissociation energy and an evaluation of the BiF red emission band systems, Chem. Phys. 155 (1991) 423–433. Erratum, T. Devore, L. Brock, R. Kahlscheuer, K. Dulaney and J.L. Gole 156 (1991) 156

The structure of mixed watery clusters, B.R. Veenstra, H.C. Meijers, P.J. de Lange and J. Kommandeur 156 (1991) 157

S_1–T_1 coupling in propynal by level anticrossing spectroscopy, M. Lombardi, J.P. Pique, U. Brühlmann and J.R. Huber 156 (1991) 163

Dissociation of aliphatic hydrocarbons excited by electrons: translational energy distributions of the excited hydrogen atom, T. Ogawa, T. Tsuboi and K. Nakashima 156 (1991) 465

Dissociation of hydrogen sulfide in e–H_2S collisions: translational energy distribution of $H^*(n=4)$, T. Ogawa, M. Tsukada and K. Nakashima 156 (1991) 473

State-to-state cross sections for rotational excitation of ortho- and para-NH_3 by He and H_2, J. Schleipen and J.J. ter Meulen 156 (1991) 479

Optothermal-detected microwave-sideband CO_2-laser spectroscopy of NCH–NH_3, G.T. Fraser, A.S. Pine, W.A. Kreiner and R.D. Suenram 156 (1991) 523

The vibrational constant of the $O_2^{2+}X\,^1\Sigma_g^+$ state from the dissociative decay of $n=3,4$ Rydberg states in O_2^+, W.J. van der Zande 157 (1991) 287
The benzene dication: energies of excited states determined by double-charge-transfer spectroscopy using OH^+ and F^+ projectile ions, W.J. Griffiths and F.M. Harris 157 (1991) 299
Excited states of hydrogen emitted from a graphite diffusion source: Arrhenius behaviour, E. Wallin and L. Holmlid 159 (1992) 313
The dissociation dynamics of low lying triplet states in butane and butene molecules, J.H.M. Beijersbergen, C.G. de Koster, W.J. van der Zande, P.G. Kistemaker and J. Los 160 (1992) 151

Time-resolved experiments

Determination of the radiative lifetimes of nine ion-pair states of I_2, P.J. Jewsbury, K.P. Lawley, T. Ridley, F.F. Al-Adel, P.R.R. Langridge-Smith and R.J. Donovan 151 (1991) 103
Trans–cis photoisomerization mechanism of carbocyanines: experimental check of theoretical models, G. Ponterini and F. Momicchioli 151 (1991) 111
Secondary heating effects in laser-induced fluorescence experiments, K.L. McNesby and R.D. Bates Jr. 151 (1991) 385
CO_2 laser-induced fluorescence studies of vibrational energy transfer in N_2O, K.L. McNesby and R.D. Bates Jr. 151 (1991) 401
Metal carbonyl photochemistry in organic solvents: femtosecond transient absorption and preliminary resonance Raman spectroscopy, A.G. Joly and K.A. Nelson 152 (1991) 69
Friction effect on the mechanism of photochemical redox processes in solutions, E.I. Kapinus 152 (1991) 83
Fluorescence detected level-anticrossing and spin coherence of a localized triplet state in diamond, E. van Oort and M. Glasbeek 152 (1991) 365
Production of the N_2 $(A^3\Sigma_u^+)$ metastable state by electron impact dissociative excitation of N_2O, S.M. Barnett, N.J. Mason and W.R. Newell 153 (1991) 283
Transient spectroscopy of triphenylmethane derivatives following subpicosecond irradiation, M.M. Martin, P. Plaza and Y.H. Meyer 153 (1991) 297
Xerographic dark discharge of PVK:TNF photoconductive material, J.-Y. Moisan, B. André and R. Lever 153 (1991) 305
Xerographic discharge of organic thermoplastic material, J.Y. Moisan, B. André, R. Lever and C. Servens 153 (1991) 465
Picosecond time-resolved absorption and fluorescence in the bacteriorhodopsin photocycle: vibrationally-excited species, D. Blanchard, D.A. Gilmore, T.L. Brack, H. Lemaire, D. Hughes and G.H. Atkinson 154 (1991) 155
A femtosecond study of electronic state dynamics of fucoxanthin and implications for photosynthetic carotenoid-to-chlorophyll energy transfer mechanisms, A.P. Shreve, J.K. Trautman, T.G. Owens and A.C. Albrecht 154 (1991) 171
Kinetics and magnetic field effect in geminate recombination of triplet radical pairs adsorbed onto porous glass studied by laser flash technique, P.P. Levin, I.V. Katalnikov and V.A. Kuzmin 154 (1991) 449
Triplet state IR spectroscopy of aromatic homocycles and heterocycles, H. Krumschmidt and C. Kryschi 154 (1991) 459
Excimer geometries in bichromophoric molecules: a theoretical and experimental study of 1,2-(bis-9-antrhyl)-ethane, G.D. Scholes, K.P. Ghiggino and G.J. Wilson 155 (1991) 127
Li-doped MgO as catalysts for oxidative coupling of methane: a positron annihilation study, G.H. Dai, Q.J. Yan, Y. Wang and Q.S. Liu 155 (1991) 275

A model description of charge carrier transport phenomena in organic molecular crystals. II. Perylene, E.A. Silinsh, G.A. Shlihta and A.J. Jurgis 155 (1991) 389
Energy and rotational state dependence of radiationless processes in propynal, P.R. Willmott, H. Bitto and J.R. Huber 156 (1991) 177
Magnetic field dependence of rotationally resolved excitation spectra of the $^1B_{3u}$ 0_0^0 transition of jet-cooled pyrazine, P.J. de Lange, H.Th. Jonkman and K.E. Drabe 156 (1991) 209
A time-resolved fluorescence study of electronic excitation energy transport in concentrated dye solutions, A.D. Scully, A. Matsumoto and S. Hirayama 157 (1991) 253
The effect of pressure on the dynamic quenching by oxygen of the excited singlet state of 9,10-dimethylanthracene in solution, A.D. Scully, H. Yasuda, M. Okamoto and S. Hirayama 157 (1991) 271
Relaxation of singlet molecular oxygen in the liquid and gas phase up to 154 K, M. Seidl, J. Kaa and M. Maier 157 (1991) 279
Radiative lifetimes of confined excitations in sigma-conjugated silane oligomers, J.R.G. Thorne, S.A. Williams, R.M. Hochstrasser and P.J. Fagan 157 (1991) 401
Photothermal grating spectroscopy study of nongeminate atom recombination of photodissociated iodine in liquids, X.R. Zhu and J.M. Harris 157 (1991) 409
Radiative and radiationless depopulation of the excited intramolecular charge transfer states: aryl derivatives of aromatic amines, J. Herbich and A. Kapturkiewicz 158 (1991) 143
Intramultiplet relaxation of $Cd(5^3P_2)$ induced by collisions with N_2 and CO, A. Masaki, T. Ohnuma, K. Kuwahara, H. Umemoto, Y. Wada, F. Misaizu and K. Fuke 158 (1991) 155
Protein relaxation dynamics in human myoglobin, D.G. Lambright, S. Balasubramanian and S.G. Boxer 158 (1991) 249
The dynamics of the primary event in rhodopsins revisited, A. Warshel, Z.T. Chu and J.-K. Hwang 158 (1991) 303
Fluorescence and molecular dynamics study of the internal motion of the buried tryptophan in bacteriophage T4 lysozyme: effects of temperature and alteration of nonbonded networks, D.L. Harris and B.S. Hudson 158 (1991) 353
Dynamics of the hydrate and amide groups of crystalline ribonuclease and lysozyme, M.G. Usha, J. Speyer and R.J. Wittebort 158 (1991) 487
Theoretical and experimental study on the electronic spectrum and photophysics of Michler's hydrol blue, I. Baraldi, A. Carnevali, F. Momicchioli and G. Ponterini 160 (1992) 85
Temperature dependence of cyanogen radical reactions with selected alkanes: CN reactivities towards primary, secondary and tertiary C–H bonds, D.L. Yang, T. Yu, N.S. Wang and M.C. Lin 160 (1992) 307
CN radical reactions with selected olefins in the temperature range 174–740 K, D.L. Yang, T. Yu, N.S. Wang and M.C. Lin 160 (1992) 317
Nuclear quadrupole interaction of $^{99}Mo(\beta^-)^{99}Tc$ in various molybdenum sulfur cluster compounds and thermal decomposition products of $(NH_4)_2[Mo_3S(S_2)_6]\cdot nH_2O$ ($n=0$–2), P. Mottner, A. Lerf, T. Butz, H. Knözinger, A. Müller, V. Wittneben and E. Krickemeyer 160 (1992) 327
Experimental and theoretical investigation of the reaction $CF_3+NO+M\rightarrow CF_3NO+M$ from 0.5 to 12 Torr and from 253 to 373 K, J. Masanet, F. Caralp, L. Ley and R. Lesclaux 160 (1992) 383
Sub-picosecond time-resolved IR spectroscopy of the vibrational dynamics of $Rh(CO)_2(acac)$, J.D. Beckerle, M. Casassa, R.R. Cavanagh, E.J. Heilweil and J.C. Stephenson 160 (1992) 487

Mass spectrometry

A classical study on the vibrational motion of a diatomic molecule in a collisional vibronic excitation, R.F.M. Lobo and A.M.C. Moutinho 151 (1991) 95

Photoionization mass spectrometry of kinetic energy-selected ions. An ion retarding potential difference method applied to NO^+ and O^+ from N_2O, R. Locht, G. Hagenow, K. Hottmann and H. Baumgärtel 151 (1991) 137

Hydroxonium ion formation in collisions of $H_2O^+ + D_2O$ and $D_2O^+ + H_2O$: a crossed-beam scattering study, J. Vančura and Z. Herman 151 (1991) 249

Excitation and ionization of freon molecules. II. Absolute oscillator strengths for the photoabsorption (7.5–200 eV) and the ionic photofragmentation (12.5–80 eV) of CF_3Cl, W. Zhang, G. Cooper, T. Ibuki and C.E. Brion 151 (1991) 343

Quantum effects in competitive unimolecular reactions, F. Remacle, M. Desouter-Lecomte and J.C. Lorquet 153 (1991) 201

Excitation and ionization of freon molecules. IV. Absolute oscillator strengths for the photoabsorption (6–200 eV) and the ionic photofragmentation (11.5–49 eV) of $CFCl_3$, W. Zhang, G. Cooper, T. Ibuki and C.E. Brion 153 (1991) 491

Multiphoton dissociation dynamics of highly excited states of CS_2 and CS_2 clusters, E. Patsilinakou, D. Proch and C. Fotakis 153 (1991) 503

Translational energy study of CH_3 photofragments following $^1(n,\pi^*)$ excitation of acetone, L.D. Waits, R.J. Horwitz and J.A. Guest 155 (1991) 149

The photoionization of ammonia revisited. The vibrational autoionization of NH_3 and its three isotopomers in the 10–12 eV photon energy range, R. Locht, B. Leyh, W. Denzer, G. Hagenow and H. Baumgärtel 155 (1991) 407

The structure of mixed watery clusters, B.R. Veenstra, H.C. Meijers, P.J. de Lange and J. Kommandeur 156 (1991) 157

The structure and stability of Cl_n^- clusters, $n=2$–7, G.L. Gutsev 156 (1991) 427

The vibrational constant of the $O_2^{2+}X\,^1\Sigma_g^+$ state from the dissociative decay of $n=3,4$ Rydberg states in O_2^+, W.J. van der Zande 157 (1991) 287

The benzene dication: energies of excited states determined by double-charge-transfer spectroscopy using OH^+ and F^+ projectile ions, W.J. Griffiths and F.M. Harris 157 (1991) 299

Core level photoionization mass spectroscopy of the fluoromethylsilanes, $Si(CH_3)_xF_{4-x}$ ($x=0$–4), around the Si 2p ionization edges, J.D. Bozek, K.H. Tan, G.M. Bancroft and K.J. Fu 158 (1991) 171

Characterization of the $\tilde{B}\leftarrow\tilde{X}$ transition of the chlorobenzene cation prepared in non-equilibrium rotational population distributions by resonance enhanced multiphoton ionization, F. Morlet-Savary, I. Dimicoli, C. Cossart-Magos and J.E. Parkin 159 (1992) 303

Photoionization mass spectrometry of kinetic energy-selected ions. The translational energy distribution of N^+/N_2 in the inner-shell ionization energy range, R. Locht, W. Denzer, E. Rühl and H. Baumgärtel 160 (1992) 477

X-ray, electron and neutron diffraction

An electrostatic-surface stability interpretation of the "hydrophobic" force inferred to occur between mica plates in solutions of soluble surfactants, R. Podgornik and V.A. Parsegian 154 (1991) 477

Comparative studies of the underlying local order corresponding to different radial distribution functions of disordered materials, G. Tóth and L. Pusztai 160 (1992) 405

Neutron scattering
Proton transfer dynamics in the hydrogen bond. Inelastic neutron scattering, infrared and Raman spectra of $Na_3H(SO_4)_2$, $K_3H(SO_4)_2$ and $Rb_3H(SO_4)_2$, F. Fillaux, A. Lautié, J. Tomkinson and G.J. Kearley 154 (1991) 135
Proton-transfer dynamics in the hydrogen bond. Inelastic neutron scattering, infrared and Raman spectra of $KH(CF_3COO)_2$ and $CsH(CF_3COO)_2$, F. Fillaux and J. Tomkinson 158 (1991) 113

Field emission and field ionization
Excited states of hydrogen emitted from a graphite diffusion source: Arrhenius behaviour, E. Wallin and L. Holmlid 159 (1992) 313

Measurement of macroscopic variables
Kinetics of the reactions of intrinsic and phosphorus doped polycrystalline silicon with molecular chlorine, Z.H. Walker and E.A. Ogryzlo 153 (1991) 483
Experimental determination of the range of interactions of dipole moments in a liquid, J.J. Makosz 155 (1991) 285

Objects

Bulk systems

Gases
The influence of the spin–orbit and the hyperfine interaction on the asymptotic behaviour of the $A\,^1\Sigma_u^+$ state of Na_2, H. Knöckel, T. Johr, H. Richter and E. Tiemann 152 (1991) 399
Relaxation cross sections for transfer of rotational angular momentum in a semiclassical approximation, A.V. Storozhev and M.L. Strekalov 153 (1991) 99
Heavy ions in mixtures of light gases: Fokker–Planck equation and its solution, L. Ferrari 153 (1991) 115
Generalized Einstein relations for ions in molecular gases, A.D. Koutselos and E.A. Mason 153 (1991) 351
Emission of Xe:N(^{2}P) collision complexes near the N(^{2}P→^{2}D) lines, A.F. Vilesov, J. Wildt and E.H. Fink 153 (1991) 531
Absolute partial photoionization cross sections of ethylene, F.A. Grimm, T.A. Whitley, P.R. Keller and J.W. Taylor 154 (1991) 303
Vibrational energy transfer in the N_2^*–OCS system. Measurements of vibrational populations of the bending manifold in the perturbed steady state by microwave spectroscopy, L.B. Favero, M.C. Righetti and P.G. Favero 155 (1991) 107
Lowest energy triplet states of group Vb hydrides: NH_3 (ND_3) and PH_3, M. Ben Arfa and M. Tronc 155 (1991) 143
Experimental and theoretical study of the N_{1s} and C_{1s} shake-up satellites in pyridine and aniline, M.P. Keane, A. Naves de Brito, N. Correia, S. Svensson and S. Lunell 155 (1991) 379
Shape resonances in low-energy electron transmission and sulfur K-shell photoabsorption spectroscopies: CH_3SH, C_2H_5SH, $(CH_3)_2S$, $(C_2H_5)_2S$, C_6H_5SH, $C_6H_5SCH_3$, CH_3SCN, CH_3NCS, SCl_2, C. Dezarnaud, M. Tronc and A. Modelli 156 (1991) 129
Methyl torsion in $C_2H_{4-n}(CH_3)_n$, $n=1$ or 2, R. Engeln and J. Reuss 156 (1991) 215
Vibrational relaxation of glyoxal in collisions with He and Ar, G.-J. Kroes and R.P.H. Rettschnick 156 (1991) 293
Ab initio calculation of the second virial coefficient of neon and the potential energy curve of Ne_2, R. Eggenberger, S. Gerber, H. Huber and D. Searles 156 (1991) 395
Zeeman effect in the two-photon excitation spectrum of the $C\,^2\Pi$ state of NO, S. Guizard, N. Shafizadeh, D. Chapoulard, M. Horani and D. Gauyacq 156 (1991) 509

Specific heat from an unsymmetrical double well potential, I.D. Feranchuk, A.P. Ulyanenkov and V.S. Kuz'min 157 (1991) 61
Ab initio quantum-chemical study of the unimolecular pyrolysis mechanisms of fluoroformic and chloroformic acid, J.S. Francisco and W.A. Ghoul 157 (1991) 89
Ab initio calculation of phosphorus NMR chemical shifts in the gauge including atomic orbital method, D.B. Chesnut and B.E. Rusiloski 157 (1991) 105
On the critical scattering phenomena of a nonpolar fluid composed of chiral molecules, E.-K. Lee, D.J. Lee and S.K. Kim 157 (1991) 135
Relaxation of singlet molecular oxygen in the liquid and gas phase up to 154 K, M. Seidl, J. Kaa and M. Maier 157 (1991) 279
Interaction between two chemical reactions in gases. The nonequilibrium effects from the Boltzmann and Fokker–Planck equations within a Lorentz gas model, A.S. Cukrowski, A.L. Kawczyński, J. Popielawski, W. Stiller and R. Schmidt 159 (1992) 39
Characterization of the $\tilde{B}\leftarrow\tilde{X}$ transition of the chlorobenzene cation prepared in non-equilibrium rotational population distributions by resonance enhanced multiphoton ionization, F. Morlet-Savary, I. Dimicoli, C. Cossart-Magos and J.E. Parkin 159 (1992) 303
Temperature dependence of cyanogen radical reactions with selected alkanes: CN reactivities towards primary, secondary and tertiary C–H bonds, D.L. Yang, T. Yu, N.S. Wang and M.C. Lin 160 (1992) 307
CN radical reactions with selected olefins in the temperature range 174–740 K, D.L. Yang, T. Yu, N.S. Wang and M.C. Lin 160 (1992) 317
Experimental and theoretical investigation of the reaction $CF_3+NO+M\rightarrow CF_3NO+M$ from 0.5 to 12 Torr and from 253 to 373 K, J. Masanet, F. Caralp, L. Ley and R. Lesclaux 160 (1992) 383
Evidence for a gauche minor-conformer of 1,3-butadiene, R. Engeln, D. Consalvo and J. Reuss 160 (1992) 427
Photoionization mass spectrometry of kinetic energy-selected ions. The translational energy distribution of N^+/N_2 in the inner-shell ionization energy range, R. Locht, W. Denzer, E. Rühl and H. Baumgärtel 160 (1992) 477

Supersonic beams

Rovibronic level structure of electronically excited acetylene ($\tilde{A}\,^1A_u$) in a supersonic jet as studied by laser-induced fluorescence and Zeeman quantum beat spectroscopy, N. Ochi and S. Tsuchiya 152 (1991) 319
The $C(^3P_J)+NO(X^2\Pi_r)\rightarrow CN(X^2\Sigma^+)+O(^3P_J)$ reaction dynamics studied at 0.06 and 0.23 eV relative translational energy in pulsed crossed supersonic molecular beams, C. Naulin, M. Costes and G. Dorthe 153 (1991) 519
The structure of mixed watery clusters, B.R. Veenstra, H.C. Meijers, P.J. de Lange and J. Kommandeur 156 (1991) 157
Energy and rotational state dependence of radiationless processes in propynal, P.R. Willmott, H. Bitto and J.R. Huber 156 (1991) 177
Real-time dynamics of vibrational predissociation in anthracene–Ar_n ($n=1,2,3$), A. Heikal, L. Bañares, D.H. Semmes and A.H. Zewail 156 (1991) 231
A fluorescence characterization of the *p*-difluorobenzene–argon van der Waals complex. Energy levels, geometries and dissociation energies, M.-C. Su, H.-K. O and C.S. Parmenter 156 (1991) 261
State-to-state cross sections for rotational excitation of ortho- and para-NH_3 by He and H_2, J. Schleipen and J.J. ter Meulen 156 (1991) 479

Fluorescence excitation spectrum of 1,8-disubstituted naphthalenes in supersonic jet, T. Chakraborty and M. Chowdhury 159 (1992) 439

Liquids neat

Frequency-dependent solvent friction and torsional damping in liquid 1,2-difluoroethane, R.A. MacPhail and F.C. Monroe 152 (1991) 93

Ion solvation dynamics in an interaction-site model solvent, F.O. Raineri, Y. Zhou, H.L. Friedman and G. Stell 152 (1991) 201

Structure and dynamics of polar liquids: a molecular dynamics investigation of N,N-dimethyl formamide, S. Yashonath and C.N.R. Rao 155 (1991) 351

Effects of solvent viscoelasticity in the solvation dynamics of an ion in a dense dipolar liquid, A. Chandra and B. Bagchi 156 (1991) 323

Relaxation of singlet molecular oxygen in the liquid and gas phase up to 154 K, M. Seidl, J. Kaa and M. Maier 157 (1991) 279

Test of effective pair potential models by molecular dynamics simulation on liquid OCS, J. Samios, H. Stassen and T. Dorfmüller 160 (1992) 33

Liquid mixtures and solutions

Ab initio molecular orbital treatment of hydroxylamine–X^+–water and hydroxylamine–X^+–ammonia (X=H, Li) clusters, M. Alcamí, O. Mó and M. Yáñez 151 (1991) 21

Symmetry and magnetic vibrational circular dichroism spectra of a doubly degenerate vibration and its combinations with non-degenerate vibrational modes, M. Pawlikowski and O. Sonnich Mortensen 151 (1991) 73

Picosecond photodissociation and geminate radical recombination in alkane solutions of tetraphenylhydrazine, M.G. Hyde and G.S. Beddard 151 (1991) 239

An exact theory of friction for reactive collisions in a solvent using an interaction representation, D.M. Charutz and R.D. Levine 152 (1991) 31

Nonexponential solvation dynamics of simple liquids and mixtures, W. Jarzeba, G.C. Walker, A.E. Johnson and P.F. Barbara 152 (1991) 57

Metal carbonyl photochemistry in organic solvents: femtosecond transient absorption and preliminary resonance Raman spectroscopy, A.G. Joly and K.A. Nelson 152 (1991) 69

Friction effect on the mechanism of photochemical redox processes in solutions, E.I. Kapinus 152 (1991) 83

Frequency-dependent solvent friction and torsional damping in liquid 1,2-difluoroethane, R.A. MacPhail and F.C. Monroe 152 (1991) 93

Solvent cage effects and chemical dynamics in liquids, F. Patron and S.A. Adelman 152 (1991) 121

Solvent effect on activated rate processes: on the validity of the GLE approach, G. Tarjus and D. Kivelson 152 (1991) 153

Chemical reaction rates and solvation dynamics in electrolyte solutions: ion atmosphere friction, G. van der Zwan and J.T. Hynes 152 (1991) 169

Outer-sphere electron-transfer reactions in model molecular solvents: the mean spherical approximation, Y. Zhou, H.L. Friedman and G. Stell 152 (1991) 185

Velocity dependence of friction, S.-B. Zhu, S. Singh, J. Lee and G.W. Robinson 152 (1991) 221

The solvated electron in an electrolyte solution, V.D. Lakhno and O.V. Vasil'ev 153 (1991) 147

Near- and non-resonant (VV) energy transfer between molecules dissolved in liquid krypton: a comparison with liquid argon, J.J. Andrew, D.C. McDermott, S.P. Mills and C.J.S.M. Simpson 153 (1991) 247

Transient spectroscopy of triphenylmethane derivatives following subpicosecond irradiation, M.M. Martin, P. Plaza and Y.H. Meyer 153 (1991) 297
Theory of multiquantum optically detected ESR spectra of radical pairs. I. General theory. Resonances in parallel radio-frequency field, V.A. Morozov and A.B. Doktorov 153 (1991) 313
Theory of multiquantum optically detected ESR spectra of radical pairs. II. Resonances in perpendicular radio-frequency field, V.A. Morozov and A.B. Doktorov 153 (1991) 333
Electron spin exchange in micellized radical pairs. I. ^{13}C low field chemically induced dynamic nuclear polarization (CIDNP) and ^{13}C radio frequency stimulated nuclear polarization (SNP), I.A. Shkrob, V.F. Tarasov and E.G. Bagryanskaya 153 (1991) 427
Electron spin exchange in micellized radical pairs. II. Magnetic field and magnetic isotope effects in multinuclear pairs, I.A. Shkrob, V.F. Tarasov and A.L. Buchachenko 153 (1991) 443
On the solution of the Debye–Smoluchowski equation with a Coulomb potential. III. The case of a Boltzmann initial distribution and a perfectly absorbing sink, S.D. Traytak 154 (1991) 263
Photochromic thiophenefulgides. Photokinetics of two isopropyl derivatives, K. Ulrich, H. Port, H.C. Wolf, J. Wonner, F. Effenberger and H.-D. Ilge 154 (1991) 311
The two-dimensional electrolytic solution in the hypernetted chain approximation, W. Chung and S.S. Mak 155 (1991) 19
Three-time autocorrelation function of the power associated with a Gaussian random process, L. Song and J.M. Schurr 155 (1991) 63
Spatial dispersion of electron transfer probability, A.I. Burshtein, P.A. Frantsuzov and A.A. Zharikov 155 (1991) 91
Potential of mean force by constrained molecular dynamics: a sodium chloride ion-pair in water, E. Guàrdia, R. Rey and J.A. Padró 155 (1991) 187
Monte Carlo and mean field studies of a polyelectrolyte in salt solution, C.E. Woodward and B. Jönsson 155 (1991) 207
Experimental determination of the range of interactions of dipole moments in a liquid, J.J. Makosz 155 (1991) 285
Theory of diffusion-influenced fluorescence quenching: dependence of the Stern–Volmer curve on light intensity, S. Lee, M. Yang, K.J. Shin, K.Y. Choo and D. Lee 156 (1991) 339
Zinc ion in water: intermolecular potential with approximate three-body correction and Monte Carlo simulation, Y.P. Yongyai, S. Kokpol and B.M. Rode 156 (1991) 403
Optically detected magnetic resonance study of the phosphorescent states of trans-2,2′-bipyridine, metal-free cis-2,2′-bipyridine and $[Zn(bpy)]^{2+}$, M. Yagi, B.D. Schlyer and A.H. Maki 157 (1991) 209
Fluorescence analysis of two new TICT systems: 10-cyano-9,9′-bianthryl (CBA) and 10,10′-dicyano-9,9′-bianthryl (DCBA), S. Müller and J. Heinze 157 (1991) 231
The effect of pressure on the dynamic quenching by oxygen of the excited singlet state of 9,10-dimethylanthracene in solution, A.D. Scully, H. Yasuda, M. Okamoto and S. Hirayama 157 (1991) 271
Molecular dynamics simulations of water–methanol mixtures, G. Pálinkás, E. Hawlicka and K. Heinzinger 158 (1991) 65
Charged substituents and the effect of their electric field on the electronic spectra of some aminocoumarins, S.I. Druzhinin, B.D. Bursulaya and B.M. Uzhinov 158 (1991) 137
Radiative and radiationless depopulation of the excited intramolecular charge transfer states: aryl derivatives of aromatic amines, J. Herbich and A. Kapturkiewicz 158 (1991) 143
Chemical potential, partial enthalpy and partial volume of mixtures by *NPT* molecular dynamics, D.M. Heyes 159 (1992) 149

Solvatochromatic shifts studied by multi-configuration self-consistent reaction field theory. Application to azabenzenes, H. Ågren, S. Knuts, K.V. Mikkelsen and H.J.Aa. Jensen 159 (1992) 211
^{23}Na relaxation in DNA solutions. Influence of intercalation on correlation times and coupling constants, M. Hald and J.P. Jacobsen 159 (1992) 257
Quantum-chemical calculations of the hydration energies of organic cations and anions in the framework of a continuum solvent approximation, G.E. Chudinov, D.V. Napolov and M.V. Basilevsky 160 (1992) 41
Principal-component self-modeling analysis of fluorescence for some trans-diarylethylenes. A comparison with kinetic analysis, A. Spalletti, G. Bartocci, F. Masetti, U. Mazzucato and G. Cruciani 160 (1992) 131
Theory of geminate recombination of radical pairs with instantaneously changing spin Hamiltonian. I. General theory and kinematic approximation, A.B. Doktorov, S.A. Mikhailov and P.A. Purtov 160 (1992) 223
Theory of geminate recombination of radical pairs with instantaneously changing spin-Hamiltonian. II. Method of summation of re-encounter contributions, A.B. Doktorov, S.A. Mikhailov and P.A. Purtov 160 (1992) 239
Measurement of quadratic hyperpolarizabilities of unsymmetrical donor–acceptor bi- and polyaryls: effect of size and torsion angle of aryl units, G. Puccetti, I. Ledoux, J. Zyss, A. Jutand and C. Amatore 160 (1992) 467
Sub-picosecond time-resolved IR spectroscopy of the vibrational dynamics of $Rh(CO)_2(acac)$, J.D. Beckerle, M. Casassa, R.R. Cavanagh, E.J. Heilweil and J.C. Stephenson 160 (1992) 487

Crystals

A Zeeman level crossing study of the symmetry of the potential hindering the torsional oscillator CH_3, W.T. Sobol, I.G. Cameron and M.M. Pintar 152 (1991) 337
Ferromagnetism of charge-transfer crystals, A.L. Tchougreeff and I.A. Misurkin 153 (1991) 371
Proton transfer dynamics in the hydrogen bond. Inelastic neutron scattering, infrared and Raman spectra of $Na_3H(SO_4)_2$, $K_3H(SO_4)_2$ and $Rb_3H(SO_4)_2$, F. Fillaux, A. Lautié, J. Tomkinson and G.J. Kearley 154 (1991) 135
Unusual features in the polarised single crystal electronic spectrum of $(NH_4)_2[V(H_2O)_6](SO_4)_2$: analysis of Fano antiresonance structure and bonding in the $[V(H_2O)_6]^{2+}$ complex, R.G. McDonald, R. Stranger, M.A. Hitchman and P.W. Smith 154 (1991) 179
Lattice dynamics of the orthorhombic phase of $KClO_4$: Ewald's method in molecular coordinates, G.F. Signorini, R. Righini and V. Schettino 154 (1991) 245
Energy levels of Cr^{3+} ions in C_{3i} sites of $Y_3Al_5O_{12}$, C.A. Morrison, J.B. Gruber and M.E. Hills 154 (1991) 437
High pressure study of intermolecular resonance interaction in a naphthalene crystal, K.P. Meletov 154 (1991) 469
Li-doped MgO as catalysts for oxidative coupling of methane: a positron annihilation study, G.H. Dai, Q.J. Yan, Y. Wang and Q.S. Liu 155 (1991) 275
A model description of charge carrier transport phenomena in organic molecular crystals. II. Perylene, E.A. Silinsh, G.A. Shlihta and A.J. Jurgis 155 (1991) 389
On the elastic properties of lithium, sodium and potassium oxide. An ab initio study, R. Dovesi, C. Roetti, C. Freyria-Fava, M. Prencipe and V.R. Saunders 156 (1991) 11
Molecular dynamics simulation of crystalline imidazole, S. Besnainou, G. Cardini and D.A. Dows 156 (1991) 71

^{14}N NQR investigation of some thermochromic and photochromic salicylideneanilines and related compounds, E. Hadjoudis, F. Milia, J. Seliger, V. Zagar and R. Blinc 156 (1991) 149
Nodal configurations and many-body energies in Li_3^{3+}, F_3^{3-}, $Li_2^{2+}F^-$ and $Li^+F_2^{2-}$ ions at crystal and cluster geometries, A.S. Shalabi 156 (1991) 359
Far-infrared perturbation of electron tunneling in reaction centers?, R.H. Austin, M.K. Hong, C. Moser and J. Plombon 158 (1991) 473
Two-dimensional trajectories of tunneling in the symmetric double-well potential, V.A. Benderskii, V.I. Goldanskii and D.E. Makarov 159 (1992) 29
Nuclear quadrupole interaction of $^{99}Mo(\beta^-)^{99}Tc$ in various molybdenum sulfur cluster compounds and thermal decomposition products of $(NH_4)_2[Mo_3S(S_2)_6]\cdot nH_2O$ (n=0–2), P. Mottner, A. Lerf, T. Butz, H. Knözinger, A. Müller, V. Wittneben and E. Krickemeyer 160 (1992) 327
Computational experiments on the intramolecular energy flow in macromolecules, B.G. Sumpter and D.W. Noid 160 (1992) 393

–neat
Time-resolved relaxation of one- and two-vibron states in the rubidium perchlorate crystal, G.M. Gale and P. Schanne 151 (1991) 127
Polar phonons in SO_2 single crystal, A. Tafi, P. Procacci, E. Castellucci and P.R. Salvi 151 (1991) 205
A Zeeman level crossing study of the symmetry of the potential hindering the torsional oscillator CH_3, W.T. Sobol, I.G. Cameron and M.M. Pintar 152 (1991) 337
Model calculations of the anthracene photocurrent spectrum, P. Petelenz and D. Mucha 154 (1991) 145
Vibrational relaxation in crystal SO_2, P. Procacci, A. Tafi, L. Angeloni, R. Righini and P.R. Salvi 154 (1991) 331
Circular dichroism spectrum of gadolinium diglycolate single crystal, T. Kundu, A.K. Banerjee and M. Chowdhury 156 (1991) 95
Electronic spectra of 4-nitro-pyridine-*n*-oxide (NPO) single crystals, M. Pierre, P.L. Baldeck, D. Block, R. Georges, H.P. Trommsdorff and J. Zyss 156 (1991) 103
Two-dimensional model of charge transfer excitons in polyacene crystals, P. Petelenz and M. Slawik 157 (1991) 169
Spinning-rate depedence of ^{31}P magic-angle-spinning nuclear magnetic resonance spectra in condensed phosphates, S. Hayashi and K. Hayamizu 157 (1991) 381
Interference and Fermi-resonant two-vibron bound states, P. Schanne and G.M. Gale 159 (1992) 1

–mixed
Triplet electron–proton cross-polarization by satisfying a modified Hartmann–Hahn condition, R.H. Fritsch, H. Brunner and K.H. Hausser 151 (1991) 261
Resonant two-photon ionization of phenol in methylene chloride doped solid argon using 248 nm KrF laser and 254 nm Hg lamp radiation, a comparative study. The UV/VIS absorption spectrum of phenol radical cation, K. Kesper, F. Diehl, J.G.G. Simon, H. Specht and A. Schweig 153 (1991) 511
The optical spectrum of $Ba_2Zn[Cu]F_6$, D. Reinen, G. Steffen, M.A. Hitchman, H. Stratemeier, L. Dubicki, E.R. Krausz, M.J. Riley, H.E. Mathies, K. Recker and F. Wallrafen 155 (1991) 117
Laser excitation and resolved emission spectra of supersonically cooled aluminum dimer, M.F. Cai, C.C. Carter, T.A. Miller and V.E. Bondybey 155 (1991) 233
A cluster model of the charge transfer interaction between an impurity and the host molecular crystal, P. Petelenz and A. Eilmes 155 (1991) 247

Electronic spectra and proton transfer in the phenol/$(NH_3)_n$ clusters in argon matrices, C. Crépin and A. Tramer 156 (1991) 281
Singlet excitation energy transfer in tetracene doped *p*-terphenyl single crystals, A. Krüger, C. Kryschi, L. Valkunas and D. Schmid 157 (1991) 243
Optical and ODMR spectroscopy of an induced triplet X-trap in 1,4-dibromobenzene single crystals, B. Stein, F. Rothamel, T. Kirski, J. Kolenda and C. von Borczyskowski 159 (1992) 269
Electronic spectra of the naphthyridines: 2,7-naphthyridine, P. Wormell and A.R. Lacey 160 (1992) 55

Glasses
Triplet state IR spectroscopy of aromatic homocycles and heterocycles, H. Krumschmidt and C. Kryschi 154 (1991) 459
New Monte Carlo simulations of many-particle stochastic dynamics: growth of correlations and local self-ordering during annihilation of like particles, R. Brown and N.A. Efremov 155 (1991) 357
Laser-initiated chain reactions and microexplosions in solid solutions of methylcyclopropane and chlorine, T.J. Tague Jr. and C.A. Wight 156 (1991) 141
Absorption spectra of a solvated electron in ethers, H. Abramczyk and J. Kroh 157 (1991) 373
Diffusion of molecular oxygen in pairs (anthracene–O_2) in glassy matrices, V.V. Korolev, D.G. Sushkov and N.M. Bazhin 158 (1991) 129
Protein relaxation dynamics in human myoglobin, D.G. Lambright, S. Balasubramanian and S.G. Boxer 158 (1991) 249
A molecular dynamics simulation of the C-terminal fragment of the L7/L12 ribosomal protein in solution, V. Daggett and M. Levitt 158 (1991) 501

Liquid crystals
An electrostatic-surface stability interpretation of the "hydrophobic" force inferred to occur between mica plates in solutions of soluble surfactants, R. Podgornik and V.A. Parsegian 154 (1991) 477

Polymers
Xerographic dark discharge of PVK:TNF photoconductive material, J.-Y. Moisan, B. André and R. Lever 153 (1991) 305
Resonant degenerate four wave mixing and scaling laws for saturable absorption in thin films of conjugated polymers and Rhodamine 6G, C. Bubeck, A. Kaltbeitzel, A. Grund and M. LeClerc 154 (1991) 343
Motion and geminal recombination of charged carriers in highly anisotropic three-dimensional systems (Onsager theory), G.A. Vinogradov, V.N. Likhachev and A.A. Ovchinnikov 154 (1991) 367
On the disordered distribution of defects in transpolyacetylene, F.C. Lavarda, D.A. dos Santos, D.S. Galvão and B. Laks 155 (1991) 1
The treatment of electron correlation in aperiodic systems. IV. Exciton bands and double ionization potentials, C.-M. Liegener 157 (1991) 183
On the fluorescence depolarization in bis-(N-carbazolyl) compounds, M. Hennecke and H.F. Kauffmann 157 (1991) 391
Radiative lifetimes of confined excitations in sigma-conjugated silane oligomers, J.R.G. Thorne, S.A. Williams, R.M. Hochstrasser and P.J. Fagan 157 (1991) 401
Temperature dependence of the fluorescence spectra of poly-N-vinylcarbazole films from 300 to 550 K: evidence for monomer emission, G. Giro and G. Orlandi 160 (1992) 145

The electronic structure of poly(*p*-phenylene vinylene), N. Sato, M. Lögdlund, R. Lazzaroni, W.R. Salaneck, J.-L. Brédas, D.D.C. Bradley, R.H. Friend and K.E. Ziemelis 160 (1992) 299

Semiconductors

Kinetics of the reactions of intrinsic and phosphorus doped polycrystalline silicon with molecular chlorine, Z.H. Walker and E.A. Ogryzlo 153 (1991) 483

A theoretical investigation of the hyperfine properties of normal and anomalous muonium in elemental semiconductors: diamond, silicon and germanium, M. Casarin, G. Granozzi, E. Tondello and A. Vittadini 154 (1991) 385

On the photo-sensitized injection of electrons into SnO_2 from cyanine dyes incorporated in Langmuir–Blodgett films, G. Biesmans, M. Van der Auweraer, C. Cathry, F.C. De Schryver, Y. Yonezawa and T. Sato 160 (1992) 97

Metals and alloys

Theoretical study of the electronic states of BeLi and Be_2^+, I. Fischer, V.E. Bondybey, P. Rosmus and H.-J. Werner 151 (1991) 295

Local density functional study of the structural and electronic properties of C_{60} and XC_{60} (X=K,Rb,Cs), L. Ye, A.J. Freeman and B. Delley 160 (1992) 415

Thin films

Resonant degenerate four wave mixing and scaling laws for saturable absorption in thin films of conjugated polymers and Rhodamine 6G, C. Bubeck, A. Kaltbeitzel, A. Grund and M. LeClerc 154 (1991) 343

A time-resolved fluorescence study of electronic excitation energy transport in concentrated dye solutions, A.D. Scully, A. Matsumoto and S. Hirayama 157 (1991) 253

Temperature dependence of the fluorescence spectra of poly-N-vinylcarbazole films from 300 to 550 K: evidence for monomer emission, G. Giro and G. Orlandi 160 (1992) 145

UV photoemission spectroscopic studies on molecular aggregation of triphenylamines dispersed in polycarbonate thin films, N. Sato and M. Yoshikawa 160 (1992) 289

Local density functional study of the structural and electronic properties of C_{60} and XC_{60} (X=K,Rb,Cs), L. Ye, A.J. Freeman and B. Delley 160 (1992) 415

Surfaces

Core excitation-induced photodesorption of molecular and fragment ions from CO adsorbates on metal surfaces, R. Treichler, W. Wurth, W. Riedl, P. Feulner and D. Menzel 153 (1991) 259

Polyatomic fluids near solid surfaces: a weighted-density-functional approach, T.A. Cherepanova and A.V. Stekolnikov 154 (1991) 41

Kinetics and magnetic field effect in geminate recombination of triplet radical pairs adsorbed onto porous glass studied by laser flash technique, P.P. Levin, I.V. Katalnikov and V.A. Kuzmin 154 (1991) 449

The influence of physisorption and the Eley–Rideal mechanism on a surface reaction: $CO+O_2$, J. Mai and W. von Niessen 156 (1991) 63

A theoretical study of the chemisorption of methane on a Ni(100) surface, O. Swang, K. Faegri Jr., O. Gropen, U. Wahlgren and P. Siegbahn 156 (1991) 379

On the photo-sensitized injection of electrons into SnO_2 from cyanine dyes incorporated in Langmuir–Blodgett films, G. Biesmans, M. Van der Auweraer, C. Cathry, F.C. De Schryver, Y. Yonezawa and T. Sato 160 (1992) 97

Lie algebraic approach to scattering of molecules from a solid surface, S. Lin, X. Yi and L. Cai 160 (1992) 163
Local density functional study of the structural and electronic properties of C_{60} and XC_{60} (X=K,Rb,Cs), L. Ye, A.J. Freeman and B. Delley 160 (1992) 415

Low-dimensional materials
Ferromagnetism of charge-transfer crystals, A.L. Tchougreeff and I.A. Misurkin 153 (1991) 371
Material properties of low-dimensional charge-transfer salts. I. Charge fluctuations in systems with stronger electronic correlations, M.C. Böhm and A. Staib 155 (1991) 27
Material properties of low-dimensional charge-transfer salts. II. Mode-softening, Peierls transitions and van Hove singularities, M.C. Böhm 155 (1991) 49
Hole pairing on oxygen sites in high-T_c copper–oxide superconductors induced by an effective exchange interaction: a theoretical and numerical investigation on planar lattices, A. Ferretti and A. Lami 155 (1991) 179
Scaling the WCA reference system for two-dimensional Lennard-Jones fluids, F. Cuadros and A. Mulero 156 (1991) 33
Pressure dependence of the polarized reflectance spectrum of a solid charge-transfer complex, perylene-hexacyanobutadiene (HCBD), T. Ida, K. Yakushi, H. Kuroda, H. Yamochi and G. Saito 156 (1991) 113
Pressure dependence of the polarized reflectance spectrum of a solid charge-transfer complex, perylene-hexacyanobutadiene (HCBD), Chem. Phys. 156 (1991) 113–122. Erratum, T. Ida, K. Yakushi, H. Kuroda, H. Yamochi and G. Saito 157 (1991) 305
The radial distribution function for two-dimensional Lennard-Jones fluids: computer simulation results, F. Cuadros and A. Mulero 159 (1992) 89
A validity test of the WCA perturbation theory for two-dimensional Lennard-Jones fluids, F. Cuadros and A. Mulero 160 (1992) 375

Dielectrics
Ion solvation dynamics in an interaction-site model solvent, F.O. Raineri, Y. Zhou, H.L. Friedman and G. Stell 152 (1991) 201
A dipolar chain model for the electrostatics of transmembrane ion channels, M.B. Partenskii, M. Cai and P.C. Jordan 153 (1991) 125
Xerographic discharge of organic thermoplastic material, J.Y. Moisan, B. André, R. Lever and C. Servens 153 (1991) 465

Plasmas
Dissociative excitation of hydrogen in rf and dc glow discharges through H_2, S.B. Vrhovac, S.B. Radovanov, S.A. Bzenić, Z.Lj. Petrović and B.M. Jelenković 153 (1991) 233
Calculation of the inner shell excitation spectra and estimation of the electron scattering and dissociative attachment resonance energies of SF_6, SO_2, SF_2O, SF_2O_2, SF_4, SF_4O and S_2F_{10}, J.A. Tossell 154 (1991) 211
Dissociation rate and $N(^4S)$ atom concentrations in a N_2 glow-discharge, J. Loureiro 157 (1991) 157

Biological systems
A dipolar chain model for the electrostatics of transmembrane ion channels, M.B. Partenskii, M. Cai and P.C. Jordan 153 (1991) 125

Picosecond time-resolved absorption and fluorescence in the bacteriorhodopsin photocycle: vibrationally-excited species, D. Blanchard, D.A. Gilmore, T.L. Brack, H. Lemaire, D. Hughes and G.H. Atkinson 154 (1991) 155
A femtosecond study of electronic state dynamics of fucoxanthin and implications for photosynthetic carotenoid-to-chlorophyll energy transfer mechanisms, A.P. Shreve, J.K. Trautman, T.G. Owens and A.C. Albrecht 154 (1991) 171
A dipolar chain model for the electrostatics of transmembrane ion channels, Chem. Phys. 153 (1991) 125–131. Erratum, M.B. Partenskii, M. Cai and P.C. Jordan 154 (1991) 197
Simulation of the unstable dynamics of excitable biomembranes: properties of a cyclic electrochemical gating mechanism, K.D. Schulze 156 (1991) 43
Test-particle model potentials for hydrogen-bonded complexes: complexes formed from HCN, HF, H_2O, NH_3, $HCONH_2$, $HCONHCH_3$, guanine and cytosine, K.P. Sagarik, V. Pongpituk, S. Chaiyapongs and P. Sisot 156 (1991) 439
Hydrogen-exchange labeling study of the allosteric R-state to T-state equilibrium in methemoglobin, R.E. McKinnie, J.J. Englander and S.W. Englander 158 (1991) 283
Stabilization of α-helical secondary structure during high-temperature molecular-dynamics simulations of α-lactalbumin, P. Fan, D. Kominos, D.B. Kitchen, R.M. Levy and J. Baum 158 (1991) 295
The dynamics of the primary event in rhodopsins revisited, A. Warshel, Z.T. Chu and J.-K. Hwang 158 (1991) 303
Fluorescence and molecular dynamics study of the internal motion of the buried tryptophan in bacteriophage T4 lysozyme: effects of temperature and alteration of nonbonded networks, D.L. Harris and B.S. Hudson 158 (1991) 353
Determination of Fe–CO geometry and heme rigidity in carbonmonoxyhemoglobin using femtosecond IR spectroscopy, B. Locke, T. Lian and R.M. Hochstrasser 158 (1991) 409
Coupling of protein motion to electron transfer: molecular dynamics and stochastic quantum mechanics study of photosynthetic reaction centers, K. Schulten and M. Tesch 158 (1991) 421

Microscopic systems

Atoms

Relation between total energy and sum of orbital energies for neutral atoms, A. Nagy and N.H. March 153 (1991) 141
Doppler-free radio frequency lineshape theory for a three-level system with three allowed transitions in presence of an IR pump, S. Ghoshal and A. Datta 153 (1991) 161
Calculation of excitation energies using quasidegenerate variational perturbation theory and multireference-averaged coupled-pair functional theory, M.A. Anderson and R.J. Cave 154 (1991) 1
Quantumchemical electronegativity and hardness indices for bonded atoms, L. Komorowski and J. Lipiński 157 (1991) 45
The He–N_2 interaction revisited: a comparison of measured and computed differential cross sections, F.A. Gianturco, A. Palma and N. Sanna 158 (1991) 77
Time-dependent calculation of the energy resolved state-to-state transition probabilities for three-atom exchange reactions, M. Monnerville, P. Halvick and J.C. Rayez 159 (1992) 227
Assessment of Gaussian-weighted angular resolution functions in the comparison of quantum-mechanically calculated electron momentum distributions with experiment, P. Duffy, M.E. Casida, C.E. Brion and D.P. Chong 159 (1992) 347

Molecules (neutral and ionic)
Symmetry and magnetic vibrational circular dichroism spectra of a doubly degenerate vibration and its combinations with non-degenerate vibrational modes, M. Pawlikowski and O. Sonnich Mortensen 151 (1991) 73
Ab initio SCF study on $LiClO_4$ and Li_2SO_4 molecules: geometries and vibrational frequencies, F. Ramondo, L. Bencivenni, R. Caminiti and C. Sadun 151 (1991) 179
Outer-sphere electron-transfer reactions in model molecular solvents: the mean spherical approximation, Y. Zhou, H.L. Friedman and G. Stell 152 (1991) 185
Observation of level crossing and level anticrossing signals in the CO_2 laser Stark spectrum of POF_3 and their proposed application to electric field standards in laser Stark spectroscopy, K. Tanaka, K. Someya and T. Tanaka 152 (1991) 229
A quantum chemical study on the alternative mechanisms of the thermal cis–trans isomerization of streptocyanines, T. Krossner and F. Dietz 153 (1991) 63
Cluster structure in model electrolyte solutions, J.L.F. Abascal and P. Turq 153 (1991) 79
Doppler-free radio frequency lineshape theory for a three-level system with three allowed transitions in presence of an IR pump, S. Ghoshal and A. Datta 153 (1991) 161
Transient spectroscopy of triphenylmethane derivatives following subpicosecond irradiation, M.M. Martin, P. Plaza and Y.H. Meyer 153 (1991) 297
The structures and stability of the $Si_3H_6^{2+}$ dications. A theoretical study, T. Kudo and S. Nagase 153 (1991) 379
The correlated molecular electrostatic potential and electric field of 2(1H)-pyrimidone and 2-hydroxypyrimidine, A. Leś and L. Adamowicz 153 (1991) 409
Resonant two-photon ionization of phenol in methylene chloride doped solid argon using 248 nm KrF laser and 254 nm Hg lamp radiation, a comparative study. The UV/VIS absorption spectrum of phenol radical cation, K. Kesper, F. Diehl, J.G.G. Simon, H. Specht and A. Schweig 153 (1991) 511
Quasiclassical trajectory study of the two channels of the F+ICl system: effect of the collisional energy, I. Urrecha, I. Serna and J. Iturbe 154 (1991) 85
Isomerization and unimolecular rearrangement channels of dithioformic acid, Y. Tao 154 (1991) 221
Lattice dynamics of the orthorhombic phase of $KClO_4$: Ewald's method in molecular coordinates, G.F. Signorini, R. Righini and V. Schettino 154 (1991) 245
On the validity of the RWA for steady state and temporal populations of molecular states involved in IR multi-photon excitations, S. Nakai and W.J. Meath 154 (1991) 349
Semiempirical electrostatic polarization model of the ionic bonding in alkali and alkaline earth hydroxides and halides, J.M. Mestdagh and J.P. Visticot 155 (1991) 79
Translational energy study of CH_3 photofragments following $^1(n,\pi^*)$ excitation of acetone, L.D. Waits, R.J. Horwitz and J.A. Guest 155 (1991) 149
Core–valence correlation effects on some Cu clusters, H. Åkeby and L.G.M. Pettersson 155 (1991) 197
Dissociative excitation of SiH_4 by electron impact: emission cross sections for the hydrogen Lyman series, S. Tsurubuchi, K. Motohashi, S. Matsuoka and T. Arikawa 155 (1991) 401
Total ionization cross sections for $Ne^{**}\{(2p)^5(3p); J=3\}$-molecule systems: absolute values and polarization effects, J.P.J. Driessen, M.P.I. Manders, F.J.M. van de Weijer, G.J. Sandker, W. Boom, H.C.W. Beijerinck and B.J. Verhaar 155 (1991) 447
New mechanism for the vibrational mode-specific proton-transfer reaction $NH_3^+(v)+NH_3 \rightarrow NH_2+NH_4$. Tachibana, T. Suzuki, N. Yoshida, Y. Teramoto and T. Yamabe 156 (1991) 79
^{14}N NQR investigation of some thermochromic and photochromic salicylideneanilines and related compounds, E. Hadjoudis, F. Milia, J. Seliger, V. Zagar and R. Blinc 156 (1991) 149

Test-particle model potentials for hydrogen-bonded complexes: complexes formed from HCN, HF, H_2O, NH_3, $HCONH_2$, $HCONHCH_3$, guanine and cytosine, K.P. Sagarik, V. Pongpituk, S. Chaiyapongs and P. Sisot 156 (1991) 439
Intramolecular dynamics of the C_4H_8NH radical cation. An application of the anisotropic exchange theory for powder ESR lineshapes, L. Sjöqvist, N.P. Benetis, A. Lund and J. Maruani 156 (1991) 457
Optothermal-detected microwave-sideband CO_2-laser spectroscopy of NCH–NH_3, G.T. Fraser, A.S. Pine, W.A. Kreiner and R.D. Suenram 156 (1991) 523
Quantumchemical electronegativity and hardness indices for bonded atoms, L. Komorowski and J. Lipiński 157 (1991) 45
Ab initio quantum-chemical study of the unimolecular pyrolysis mechanisms of fluoroformic and chloroformic acid, J.S. Francisco and W.A. Ghoul 157 (1991) 89
Variational approach to quantum dynamics: a simple application to molecular photodissociation, G.P. Arrighini, N. Durante and C. Guidotti 157 (1991) 365
Many-body calculation of the valence photoemission spectrum of ferrocene, M. Ohno, W. von Niessen and J. Schüle 158 (1991) 1
The structure and stability of S_2F_{10} and S_2F_{11} and their anions, G.L. Gutsev 158 (1991) 33
Ab initio study on the coordination structures of $M^+XY_3^-$ and $M^+XY_4^-$ ion pairs, F. Ramondo, L. Bencivenni and V. Di Martino 158 (1991) 41
The He–N_2 interaction revisited: a comparison of measured and computed differential cross sections, F.A. Gianturco, A. Palma and N. Sanna 158 (1991) 77
Diffusion of molecular oxygen in pairs (anthracene–O_2) in glassy matrices, V.V. Korolev, D.G. Sushkov and N.M. Bazhin 158 (1991) 129
MO LCAO analysis of the vibronic instability of the $CuCl_5^{3-}$ trigonal bipyramidal configuration. Critical view on the angular overlap model in vibronic problems, V.Z. Polinger, N.N. Gorinchoi and I.B. Bersuker 159 (1992) 75
The radial distribution function for two-dimensional Lennard-Jones fluids: computer simulation results, F. Cuadros and A. Mulero 159 (1992) 89
Variational approach to continuum orbitals in a spline basis: an application to H_2^+ photoionization, M. Brosolo and P. Decleva 159 (1992) 185
Ab initio study of the vibrational structure of the X^2A_1 and A^2B_1 electronic states of CH_2^+, W. Reuter and S.D. Peyerimhoff 160 (1992) 11
The Pariser–Parr–Pople model for trans-polyenes. II. Parametrization and ground state dynamics, W. Förner 160 (1992) 189
Structural and spectral consequences of ion-pairing. VI. $BO_2^-Li^+$ and $BO_2^-Na^+$, J.S. Francisco and I.H. Williams 160 (1992) 255
The formulae for calculation of *g*-tensor shifts in third-order perturbation theory, E.N. Heifets 160 (1992) 363

–diatomic

Theoretical study of the spectroscopy of Al_2^+, M. Rosi, C.W. Bauschlicher Jr. and S.R. Langhoff 151 (1991) 1
Calculation of the vibrational frequency and line strength versus applied field of carbon monoxide, J.L. Andrés, M. Duran, A. Lledós and J. Bertrán 151 (1991) 37
Determination of the radiative lifetimes of nine ion-pair states of I_2, P.J. Jewsbury, K.P. Lawley, T. Ridley, F.F. Al-Adel, P.R.R. Langridge-Smith and R.J. Donovan 151 (1991) 103
Optical potentials by the complex coordinate method, N. Rom, N. Lipkin and N. Moiseyev 151 (1991) 199

Spectroscopy and relaxation dynamics of metastable electronically excited states of iodine in rare gas matrices, M. Macler and M.C. Heaven 151 (1991) 219
Quenching and rotational transfer rates in the $v'=0$ manifold of $OH(A^2\Sigma^+)$, J. Burris, J. Butler, T. McGee and W. Heaps 151 (1991) 233
Theoretical study of the electronic states of BeLi and Be_2^+, I. Fischer, V.E. Bondybey, P. Rosmus and H.-J. Werner 151 (1991) 295
Anomalous structure in the $A^6\Sigma^+$–$X^6\Sigma^+$ transition of MnO caused by interference between two internal hyperfine perturbations, A.G. Adam, Y. Azuma, H. Li, A.J. Merer and C. Thambir 152 (1991) 391
The influence of the spin–orbit and the hyperfine interaction on the asymptotic behaviour of the $A^1\Sigma_u^+$ state of Na_2, H. Knöckel, T. Johr, H. Richter and E. Tiemann 152 (1991) 399
Theoretical study of the spectroscopy of the alkali oxides LiO, NaO, and KO, S.R. Langhoff, H. Partridge and C.W. Bauschlicher Jr. 153 (1991) 1
Relaxation cross sections for transfer of rotational angular momentum in a semiclassical approximation, A.V. Storozhev and M.L. Strekalov 153 (1991) 99
Estimation of the integral cross section for dissociative excitation of F_2 by electron impact, D.C. Cartwright, P.J. Hay and S. Trajmar 153 (1991) 219
Dissociative excitation of hydrogen in rf and dc glow discharges through H_2, S.B. Vrhovac, S.B. Radovanov, S.A. Bzenić, Z.Lj. Petrović and B.M. Jelenković 153 (1991) 233
Bond formation between positively charged species. Non-adiabatic analysis and valence-bond model in the CO^{2+} case, N. Levasseur, Ph. Millie, P. Archirel and B. Levy 153 (1991) 387
Heteronuclear transition metal diatomics: the bonding and electronic structure of ScNi, YNi, ScPd and YPd, K. Faegri Jr. and C.W. Bauschlicher Jr. 153 (1991) 399
The $C(^3P_J)+NO(X^2\Pi_r)\rightarrow CN(X^2\Sigma^+)+O(^3P_J)$ reaction dynamics studied at 0.06 and 0.23 eV relative translational energy in pulsed crossed supersonic molecular beams, C. Naulin, M. Costes and G. Dorthe 153 (1991) 519
Polyatomic fluids near solid surfaces: a weighted-density-functional approach, T.A. Cherepanova and A.V. Stekolnikov 154 (1991) 41
An experimental and theoretical study of SF^{q+} ($q=1$–3) ions, K. Nagesha, V.R. Marathe and D. Mathur 154 (1991) 125
Potential curves and predissociation rates for the heavy species HBr^{2+} and DBr^{2+}, A. Banichevich, S.D. Peyerimhoff, B.A. Hess and M.C. van Hemert 154 (1991) 199
On the validity of the RWA for steady state and temporal populations of molecular states involved in IR multi-photon excitations, S. Nakai and W.J. Meath 154 (1991) 349
The generator coordinate Hartree–Fock method for molecular systems. Formalism and first applications to H_2, LiH and Li_2, H.F.M. da Costa, A.B.F. da Silva, J.R. Mohallem, A.M. Simas and M. Trsic 154 (1991) 379
Theoretical study of the $HeH(B^2\Pi)$ fluorescence and predissociation, A.B. Alekseyev, V.S. Ivanov, A.M. Pravilov and O.D. Shestakov 155 (1991) 173
Core–valence correlation effects on some Cu clusters, H. Åkeby and L.G.M. Pettersson 155 (1991) 197
On the BiF bond dissociation energy and an evaluation of the BiF red emission band systems, T.C. Devore, L. Brock, R. Kahlscheuer, K. Dulaney and J.L. Gole 155 (1991) 423
On the BiF bond dissociation energy and an evaluation of the BiF red emission band systems, Chem. Phys. 155 (1991) 423–433. Erratum, T. Devore, L. Brock, R. Kahlscheuer, K. Dulaney and J.L. Gole 156 (1991) 156
Nuclear quadrupole coupling constants of rovibrational levels of all isotopic species of BH^+ in their $X^2\Sigma^+$ and $B'^2\Sigma^+$ states, J. Vojtík, L. Češpiva, I. Paidarová and J. Šavrda 156 (1991) 369

A combining rule calculation of the van der Waals potentials of the rare-gas hydrides, K.T. Tang and J.P. Toennies 156 (1991) 413
Laser excitation of the $A^3\Sigma_u^+$, $A'^3\Delta_u$ and $c^1\Sigma_u^-$ states of molecular oxygen, J. Wildt, G. Bednarek, E.H. Fink and R.P. Wayne 156 (1991) 497
Zeeman effect in the two-photon excitation spectrum of the $C^2\Pi$ state of NO, S. Guizard, N. Shafizadeh, D. Chapoulard, M. Horani and D. Gauyacq 156 (1991) 509
Construction of bound-state potential energy curves of diatomic molecules from spectroscopic data, C.G. Diaz, F.M. Fernández and E.A. Castro 157 (1991) 35
Modified version of the trajectory surface leaking method for dynamical calculations on autoionizing atom–diatom collision systems, J. Vojtík and I. Paidarová 157 (1991) 67
Adiabatic calculations and properties of the He_2^+ molecular ion, J. Ackermann and H. Hogreve 157 (1991) 75
Singlet–triplet energy component differences in homonuclear diatomics: a multi-reference configuration interaction study of Hund's rule, K.V. Darvesh, P.D. Fricker and R.J. Boyd 157 (1991) 99
Transition probabilities for the $B^1\Delta_g$–$A^1\Pi_u$ and $B'^1\Sigma_g^+$–$A^1\Pi_u$ infrared bands of C_2. An ab initio study, P.J. Bruna and J.S. Wright 157 (1991) 111
The potential of the Na_2 $B^1\Pi_u$ state, H. Richter, H. Knöckel and E. Tiemann 157 (1991) 217
Relaxation of singlet molecular oxygen in the liquid and gas phase up to 154 K, M. Seidl, J. Kaa and M. Maier 157 (1991) 279
The vibrational constant of the $O_2^{2+}X^1\Sigma_g^+$ state from the dissociative decay of $n=3,4$ Rydberg states in O_2^+, W.J. van der Zande 157 (1991) 287
Photothermal grating spectroscopy study of nongeminate atom recombination of photodissociated iodine in liquids, X.R. Zhu and J.M. Harris 157 (1991) 409
Ground state electric properties of NaH, G.H.F. Diercksen and A.J. Sadlej 158 (1991) 9
Electric properties of ionic diatoms: BeO, G.H.F. Diercksen, A.J. Sadlej and M. Urban 158 (1991) 19
Angular momentum and rotational energy relaxation in N_2–N_2 collisions calculated from coherent and stimulated Raman spectroscopy data, S. Temkin, J.M. Thuet, L. Bonamy, J. Bonamy and D. Robert 158 (1991) 89
Collision-induced emission of $O_2(a^1\Delta_g \rightarrow X^3\Sigma_g^-)$ in the gas phase, J. Wildt, E.H. Fink, P. Biggs, R.P. Wayne and A.F. Vilesov 159 (1992) 127
Quasiclassical trajectory study of the effect of reactant rotation on the reaction $B^+ + HD \rightarrow BH^+(BD^+) + D(H)$, V. Klimo, J. Urban and J. Tiňo 159 (1992) 141
Time-dependent calculation of the energy resolved state-to-state transition probabilities for three-atom exchange reactions, M. Monnerville, P. Halvick and J.C. Rayez 159 (1992) 227
Site effects in spectra of matrix-isolated diatomic molecules: a modelling approach, M. Winter, K. Seranski and U. Schurath 159 (1992) 235
Site-resolved vibronic spectra of matrix-isolated NBr: comparison with model calculations, K. Seranski, M. Winter and U. Schurath 159 (1992) 247
Excited states of hydrogen emitted from a graphite diffusion source: Arrhenius behaviour, E. Wallin and L. Holmlid 159 (1992) 313
CuBr chemiluminescence from the $Cu^*(^2D_{3/2,5/2}) + Br_2$ reaction, P. Kowalczyk, I. Hikmet and N. Sadeghi 160 (1992) 73
Photoionization mass spectrometry of kinetic energy-selected ions. The translational energy distribution of N^+/N_2 in the inner-shell ionization energy range, R. Locht, W. Denzer, E. Rühl and H. Baumgärtel 160 (1992) 477

–small polyatomics
Electronic structure of linear form of OCuO, Y. Mochizuki, K. Tanaka and H. Kashiwagi 151 (1991) 11
Rotation–vibration energies of FHF^- and $ClHCl^-$ from high-level correlated calculations of potential energy surfaces, V. Špirko, A. Čejchan and G.H.F. Diercksen 151 (1991) 45
Photoionization mass spectrometry of kinetic energy-selected ions. An ion retarding potential difference method applied to NO^+ and O^+ from N_2O, R. Locht, G. Hagenow, K. Hottmann and H. Baumgärtel 151 (1991) 137
Estimation of electronic correlation energies and binding energies for molecules composed of first-row atoms, K. Rościszewski, M. Chaumet and P. Fulde 151 (1991) 159
The H_2O_2–NO_2^- and $H_2NO_4^-$ isomers of the nitrate anion–water complex, M. Shen, Y. Xie, H.F. Schaefer III and C.A. Deakyne 151 (1991) 187
Model study of the effect of anisotropy on the differential cross section for atom–molecule scattering: the double rainbows, R. Düren, R.K.B. Helbing and S. Milošević 151 (1991) 287
Jahn–Teller effect and dissociation from the ground state of CF_4^+, J.M. García de la Vega and E. San Fabián 151 (1991) 335
Excitation and ionization of freon molecules. II. Absolute oscillator strengths for the photoabsorption (7.5–200 eV) and the ionic photofragmentation (12.5–80 eV) of CF_3Cl, W. Zhang, G. Cooper, T. Ibuki and C.E. Brion 151 (1991) 343
Excitation and ionization of freon molecules. III. Absolute oscillator strengths for the photoabsorption (8.5–200 eV) and the ionic photofragmentation (11.5–70 eV) of CF_2Cl_2, W. Zhang, G. Cooper, T. Ibuki and C.E. Brion 151 (1991) 357
A study of the S_1 $6^1(^1A_2'')$ vibronically excited state of sym-triazine by high-resolution UV laser spectroscopy, P. Uijt de Haag, W.L. Meerts and J.T. Hougen 151 (1991) 371
Secondary heating effects in laser-induced fluorescence experiments, K.L. McNesby and R.D. Bates Jr. 151 (1991) 385
CO_2 laser-induced fluorescence studies of vibrational energy transfer in N_2O, K.L. McNesby and R.D. Bates Jr. 151 (1991) 401
Frequency-dependent solvent friction and torsional damping in liquid 1,2-difluoroethane, R.A. MacPhail and F.C. Monroe 152 (1991) 93
Avoided-crossing molecular-beam study of the torsion–rotation energy levels of CH_3CF_3, W.L. Meerts and I. Ozier 152 (1991) 241
FIR LMR spectra of FO_2: some classic examples of level anticrossing resonances, U. Bley, P.B. Davies, M. Grantz, T.J. Sears and F. Temps 152 (1991) 281
Anomalous behavior of the anticrossing density as a function of excitation energy in the C_2H_2 molecule, P. Dupré, R. Jost, M. Lombardi, P.G. Green, E. Abramson and R.W. Field 152 (1991) 293
Rovibronic level structure of electronically excited acetylene ($\tilde{A}\,^1A_u$) in a supersonic jet as studied by laser-induced fluorescence and Zeeman quantum beat spectroscopy, N. Ochi and S. Tsuchiya 152 (1991) 319
MRCI potential energy functions for the charge transfer reactions $H^+ + HCl$ $(X^1\Sigma^+) \rightarrow H + HCl^+$ $(X^2\Pi_i, A^2\Sigma^+)$, Th. Glenewinkel-Meyer, Ch. Ottinger, P. Rosmus and H.-J. Werner 152 (1991) 409
Ab initio calculations on the one- and two-photon electronic transitions of cyclopentadiene, spirononateraene, 1,4-cyclo-hexadiene, Dewar benzene, norbornadiene, and barrelene, V. Galasso 153 (1991) 13
Vibrational structure of the solvated glycine zwitterion, J.S. Alper, H. Dothe and D.F. Coker 153 (1991) 51
Trajectory capture rate coefficients for ion–quadrupolar molecule reactions, I. Mendaš and P. Milutinović 153 (1991) 73

An extended diatomics-in-molecules model for NH_2^+, R. Polák 153 (1991) 91
On the Jahn–Teller coupling of an orbital triplet with a vibrational doublet, E. Ghelichkhani and E.R. Grant 153 (1991) 133
The electronic states of the azines. IV. Pyrazine, studied by VUV absorption, near-threshold electron energy-loss spectroscopy and ab initio multi-reference configuration interaction calculations, I.C. Walker and M.H. Palmer 153 (1991) 169
The magnetizability and *g*-factor surfaces of ammonia, S.P.A. Sauer, V. Špirko and J. Oddershede 153 (1991) 189
Production of the N_2 ($A^3\Sigma_u^+$) metastable state by electron impact dissociative excitation of N_2O, S.M. Barnett, N.J. Mason and W.R. Newell 153 (1991) 283
Theoretical study of the reaction of OH with HNO, M.R. Soto, M. Page and M.L. McKee 153 (1991) 415
Excitation and ionization of freon molecules. IV. Absolute oscillator strengths for the photoabsorption (6–200 eV) and the ionic photofragmentation (11.5–49 eV) of $CFCl_3$, W. Zhang, G. Cooper, T. Ibuki and C.E. Brion 153 (1991) 491
Multiphoton dissociation dynamics of highly excited states of CS_2 and CS_2 clusters, E. Patsilinakou, D. Proch and C. Fotakis 153 (1991) 503
Anomalous behaviour of the anticrossing density as a function of excitation energy in the C_2H_2 molecule, Chem. Phys. 152 (1991) 293. Erratum, P. Dupré, R. Jost, M. Lombardi, P.G. Green, E. Abramson and R.W. Field 153 (1991) 539
Calculation of excitation energies using quasidegenerate variational perturbation theory and multireference-averaged coupled-pair functional theory, M.A. Anderson and R.J. Cave 154 (1991) 1
Theoretical study of the electronic spectrum of ammonia: generalized oscillator strength calculations for the A–X transition, L. Chantranupong, G. Hirsch, R.J. Buenker, M. Kimura and M.A. Dillon 154 (1991) 13
Polyatomic fluids near solid surfaces: a weighted-density-functional approach, T.A. Cherepanova and A.V. Stekolnikov 154 (1991) 41
Periodic orbits and quantum localization in the van der Waals systems CO–Ar, L. Zachilas and S.C. Farantos 154 (1991) 55
Connecting level statistics and reaction dynamics: mode selective decay of resonant states for HXXH-type molecules, B. Hartke and W. Karrlein 154 (1991) 63
Isomerization and unimolecular rearrangement channels of dithioformic acid, Y. Tao 154 (1991) 221
A theoretical study on the internal rotation and hyperfine structures of the ethyl radical (CH_3–CH_2), H.U. Suter and T.K. Ha 154 (1991) 227
Absolute partial photoionization cross sections of ethylene, F.A. Grimm, T.A. Whitley, P.R. Keller and J.W. Taylor 154 (1991) 303
Oxygen K-shell excitation spectroscopy of hydrogen peroxide, E. Rühl and A.P. Hitchcock 154 (1991) 323
On the validity of the RWA for steady state and temporal populations of molecular states involved in IR multi-photon excitations, S. Nakai and W.J. Meath 154 (1991) 349
Quantum kinetic energy operator for a group of particles in terms of scalar basic rotational invariant coordinates derived from a generalized Jacobi vector (GJV) description. III. A metric tensors approach, J.P. Leroy, H. Rabitz and R. Wallace 154 (1991) 395
Analytical potential energy surface for methane in terms of interatomic forces, H. Furue, J.F. LeBlanc, P.D. Pacey and J.M. Whalen 154 (1991) 425
The first ionization potentials of some MH_{k+1}^- and $M_2H_{2k+1}^-$ anions calculated by a Green's function method, A.I. Boldyrev and W. von Niessen 155 (1991) 71
Symmetry and vibronic coupling: the stereochemistry and the ground state potential surface of Cu^{2+} in five-coordination, D. Reinen and M. Atanasov 155 (1991) 157

Pulsed discharge source of supersonically cooled transient species, R. Schlachta, G. Lask, S.H. Tsay and V.E. Bondybey 155 (1991) 267
Valence-shell electron momentum distributions of cyclopropane by symmetric noncoplanar (e,2e) spectroscopy, M.P. Banjavčić, T.A. Daniels and K.T. Leung 155 (1991) 309
A vibrational study of the CD_3H molecule in the curvilinear formulation, C. Iung and C. Leforestier 155 (1991) 369
Dissociative excitation of SiH_4 by electron impact: emission cross sections for the hydrogen Lyman series, S. Tsurubuchi, K. Motohashi, S. Matsuoka and T. Arikawa 155 (1991) 401
The photoionization of ammonia revisited. The vibrational autoionization of NH_3 and its three isotopomers in the 10–12 eV photon energy range, R. Locht, B. Leyh, W. Denzer, G. Hagenow and H. Baumgärtel 155 (1991) 407
Photodissociation of CF_3I at 248 nm: kinetic energy dependence of the recoil anisotropy, P. Felder 155 (1991) 435
Vibronic coupling in Rydberg series of linear molecules, A. Staib, W. Domcke and A.L. Sobolewski 156 (1991) 21
The vibrational spectra of the monohalogenated cyclopropanes: ab initio calculations and an experimental study of fluorocyclopropane, C. Kaupert, H. Heydtmann and W. Thiel 156 (1991) 85
S_1–T_1 coupling in propynal by level anticrossing spectroscopy, M. Lombardi, J.P. Pique, U. Brühlmann and J.R. Huber 156 (1991) 163
Energy and rotational state dependence of radiationless processes in propynal, P.R. Willmott, H. Bitto and J.R. Huber 156 (1991) 177
Magnetic field dependence of rotationally resolved excitation spectra of the $^1B_{3u}$ 0_0^0 transition of jet-cooled pyrazine, P.J. de Lange, H.Th. Jonkman and K.E. Drabe 156 (1991) 209
Methyl torsion in $C_2H_{4-n}(CH_3)_n$, $n=1$ or 2, R. Engeln and J. Reuss 156 (1991) 215
Dissociation of aliphatic hydrocarbons excited by electrons: translational energy distributions of the excited hydrogen atom, T. Ogawa, T. Tsuboi and K. Nakashima 156 (1991) 465
Dissociation of hydrogen sulfide in e–H_2S collisions: translational energy distribution of $H^*(n=4)$, T. Ogawa, M. Tsukada and K. Nakashima 156 (1991) 473
Ab initio calculation of phosphorus NMR chemical shifts in the gauge including atomic orbital method, D.B. Chesnut and B.E. Rusiloski 157 (1991) 105
On the critical scattering phenomena of a nonpolar fluid composed of chiral molecules, E.-K. Lee, D.J. Lee and S.K. Kim 157 (1991) 135
Ring-puckering and internal rotation barriers in N,N′-dimethylethyleneurea, J.C. Otero, J.I. Marcos, E. López-Cantarero and A. Chacón 157 (1991) 201
Rotational distributions of $N_2O^+(\tilde{A}^2\Sigma^+)$, $CO_2^+(\tilde{A}^2\Pi_u)$ and $CS_2^+(\tilde{A}^2\Pi_u)$ produced by electron-impact ionization, I. Tokue, A. Masuda, H. Kume and Y. Ito 158 (1991) 161
Core level photoionization mass spectroscopy of the fluoromethylsilanes, $Si(CH_3)_xF_{4-x}$ ($x=0$–4), around the Si 2p ionization edges, J.D. Bozek, K.H. Tan, G.M. Bancroft and K.J. Fu 158 (1991) 171
Ab initio calculation of anharmonic force fields for the methyl, silyl, germyl, and stannyl halides, W. Schneider and W. Thiel 159 (1992) 49
A semiclassical simulation for tunneling dynamics of malonaldehyde and hydrogenoxalate anion, E. Bosch, M. Moreno and J.M. Lluch 159 (1992) 99
Quantum-classical reaction path model for chemical reactions. IV. The reaction $Cl^- + CH_3Cl \rightarrow ClCH_3 + Cl^-$, G.D. Billing 159 (1992) 109
Valence-shell electron momentum distributions and ionization energy spectra of tetramethylsilane by symmetric noncoplanar (e, 2e) spectroscopy, T. Daniels, H. Zhu, M.P. Banjavčić and K.T. Leung 159 (1992) 289

The importance of periodic orbits in analysing photodissociation resonances: the O_3 case, S.C. Farantos 159 (1992) 329
Assessment of Gaussian-weighted angular resolution functions in the comparison of quantum-mechanically calculated electron momentum distributions with experiment, P. Duffy, M.E. Casida, C.E. Brion and D.P. Chong 159 (1992) 347
A weak-mode representation of floppy molecules. I. Potential energy, C. Saint-Espès, X. Chapuisat and F. Schneider 159 (1992) 377
A weak-mode representation of floppy molecules. II. Kinetic energy and total Hamiltonian matrix, X. Chapuisat and C. Saint-Espès 159 (1992) 391
Ab-initio multiple reference double-excitation configuration-interaction ground and excited state potential curves for the $H_2N–NO_2$ decomposition in nitramine, S. Roszak and J.J. Kaufman 160 (1992) 1
Methyl tunnelling in solid diacetyl, A.M. Alsanoosi and A.J. Horsewill 160 (1992) 25
The dissociation dynamics of low lying triplet states in butane and butene molecules, J.H.M. Beijersbergen, C.G. de Koster, W.J. van der Zande, P.G. Kistemaker and J. Los 160 (1992) 151
The Pariser–Parr–Pople model for trans-polyenes. I. Ab initio and semiempirical study of the bond alternation in trans-butadiene, W. Förner 160 (1992) 173
Evidence for a gauche minor-conformer of 1,3-butadiene, R. Engeln, D. Consalvo and J. Reuss 160 (1992) 427
Absolute dipole differential oscillator strengths for inner shell spectra from high resolution electron energy loss studies of the freon molecules CF_4, CF_3Cl, CF_2Cl_2, $CFCl_3$ and CCl_4, W. Zhang, T. Ibuki and C.E. Brion 160 (1992) 435
Sub-picosecond time-resolved IR spectroscopy of the vibrational dynamics of $Rh(CO)_2(acac)$, J.D. Beckerle, M. Casassa, R.R. Cavanagh, E.J. Heilweil and J.C. Stephenson 160 (1992) 487

–aromatics

The electronically excited states of 2-phenylindole, B. Albinsson, S. Eriksson, R. Lyng and M. Kubista 151 (1991) 149
Degenerate triplet spin exchange in liquid solution studied by pulse NMR, J. Burri and H. Fischer 151 (1991) 279
Theoretical infrared spectra of large carbon clusters, D. Bakowies and W. Thiel 151 (1991) 309
Friction effect on the mechanism of photochemical redox processes in solutions, E.I. Kapinus 152 (1991) 83
Mixing of the vibrational angular momentum components of multiply degenerate vibronic states of benzene by vibrational *l*-type resonance, E. Riedle and J. Pliva 152 (1991) 375
Conformational dependence of the quadratic hyperpolarisabilities of a series of push–pull diaryl acetylenes: an experimental and computational investigation, M. Barzoukas, A. Fort, G. Klein, A. Boeglin, C. Serbutoviez, L. Oswald and J.F. Nicoud 153 (1991) 457
Photochromic thiophenefulgides. Photokinetics of two isopropyl derivatives, K. Ulrich, H. Port, H.C. Wolf, J. Wonner, F. Effenberger and H.-D. Ilge 154 (1991) 311
Triplet state IR spectroscopy of aromatic homocycles and heterocycles, H. Krumschmidt and C. Kryschi 154 (1991) 459
Excimer geometries in bichromophoric molecules: a theoretical and experimental study of 1,2-(bis-9-antrhyl)-ethane, G.D. Scholes, K.P. Ghiggino and G.J. Wilson 155 (1991) 127
Experimental and theoretical study of the N_{1s} and C_{1s} shake-up satellites in pyridine and aniline, M.P. Keane, A. Naves de Brito, N. Correia, S. Svensson and S. Lunell 155 (1991) 379

The trans-stilbene–Ar van der Waals complex. Vibrationally averaged substitution structure in its S_0 and S_1 electronic states, B.B. Champagne, D.F. Plusquellic, J.F. Pfanstiel, D.W. Pratt, W.M. van Herpen and W.L. Meerts 156 (1991) 251
The electronic states of the azines. V. Pyridazine, studied by VUV absorption, near threshold electron energy-loss spectroscopy and ab initio multi-reference configuration interaction calculations, M.H. Palmer and I.C. Walker 157 (1991) 187
Optically detected magnetic resonance study of the phosphorescent states of trans-2,2′-bipyridine, metal-free cis-2,2′-bipyridine and $[Zn(bpy)]^{2+}$, M. Yagi, B.D. Schlyer and A.H. Maki 157 (1991) 209
Fluorescence analysis of two new TICT systems: 10-cyano-9,9′-bianthryl (CBA) and 10,10′-dicyano-9,9′-bianthryl (DCBA), S. Müller and J. Heinze 157 (1991) 231
Singlet excitation energy transfer in tetracene doped *p*-terphenyl single crystals, A. Krüger, C. Kryschi, L. Valkunas and D. Schmid 157 (1991) 243
Charged substituents and the effect of their electric field on the electronic spectra of some aminocoumarins, S.I. Druzhinin, B.D. Bursulaya and B.M. Uzhinov 158 (1991) 137
Satellite lines at the ionization threshold in charge transfer systems, W. Wardermann and W. von Niessen 159 (1992) 11
Characterization of the $\tilde{B}\leftarrow\tilde{X}$ transition of the chlorobenzene cation prepared in non-equilibrium rotational population distributions by resonance enhanced multiphoton ionization, F. Morlet-Savary, I. Dimicoli, C. Cossart-Magos and J.E. Parkin 159 (1992) 303
Fluorescence excitation spectrum of 1,8-disubstituted naphthalenes in supersonic jet, T. Chakraborty and M. Chowdhury 159 (1992) 439
Electronic spectra of the naphthyridines: 2,7-naphthyridine, P. Wormell and A.R. Lacey 160 (1992) 55
On the mechanism of radiationless deactivation of rhodamines, T. López Arbeloa, F. López Arbeloa, P.H. Bartolomé and I. López Arbeloa 160 (1992) 123
Measurement of quadratic hyperpolarizabilities of unsymmetrical donor–acceptor bi- and polyaryls: effect of size and torsion angle of aryl units, G. Puccetti, I. Ledoux, J. Zyss, A. Jutand and C. Amatore 160 (1992) 467

–other large

Trans–cis photoisomerization mechanism of carbocyanines: experimental check of theoretical models, G. Ponterini and F. Momicchioli 151 (1991) 111
Theoretical infrared spectra of large carbon clusters, D. Bakowies and W. Thiel 151 (1991) 309
Picosecond Stokes shift studies of solvent friction: experimental measurements of time-dependent band shape and integrated intensity, J.D. Simon and S.-G. Su 152 (1991) 143
Acrylonitrile versus allyl cyanide: the role of electronic conjugation in high electric field condition, M. Raynaud, C. Reynaud, Y. Ellinger, G. Hennico and J. Delhalle 153 (1991) 39
Structure of MQ-NMR spin spaces under higher $\mathcal{S}_n$- and $(\mathcal{S}_n)_{\downarrow}\mathcal{G}$ symmetries. II. $\Gamma/\tilde{\Gamma}$ $(\mathcal{S}_6)_{\downarrow}\mathcal{O}$ subduced irreps for sixfold spin clusters pertaining to the molecular cage ion, $[^{11}BH]_6^{2-}$, J.P. Colpa and F.P. Temme 154 (1991) 97
Structure of MQ-NMR spin spaces under higher $\mathcal{S}_n$- and $(\mathcal{S}_n)_{\downarrow}\mathcal{G}$ symmetries. III. $\Gamma/\tilde{\Gamma}$ $((\mathcal{S}_7)_{\downarrow}D_5)$ subduced irreps for $[A]_7$ clusters pertaining to the molecular cage ion, $[^{11}BH]_7^{2-}$, F.P. Temme and J.P. Colpa 154 (1991) 111
Calculation of the inner shell excitation spectra and estimation of the electron scattering and dissociative attachment resonance energies of SF_6, SO_2, SF_2O, SF_2O_2, SF_4, SF_4O and S_2F_{10}, J.A. Tossell 154 (1991) 211
Model potentials in numerical local density functional methods, G.L. Gutsev, V.K. Gryaznov and V.A. Nasluzov 154 (1991) 291

Localization and correlation corrections in electronic interactions through single bonded hydrocarbon spacers, M. Braga, A. Broo and S. Larsson 156 (1991) 1
Circular dichroism spectrum of gadolinium diglycolate single crystal, T. Kundu, A.K. Banerjee and M. Chowdhury 156 (1991) 95
Vibrational and rotational effects on the intersystem crossing in pyrazine and pyrimidine, P. Uijt de Haag and W.L. Meerts 156 (1991) 197
Structure of MQ-NMR spin spaces under higher $\mathscr{S}_n$- and $(\mathscr{S}_n)_{\downarrow}\mathscr{G}$ symmetries. II. $\Gamma/\tilde{\Gamma}$ $(\mathscr{S}_6)_{\downarrow}\mathscr{O}$ subduced irreps for sixfold spin clusters pertaining to the molecular cage ion, $[^{11}BH]_6^{2-}$, Chem. Phys. 154 (1991) 97–110. Erratum, J.P. Colpa and F.P. Temme 156 (1991) 532
Ab initio quantum-chemical study of the unimolecular pyrolysis mechanisms of fluoroformic and chloroformic acid, J.S. Francisco and W.A. Ghoul 157 (1991) 89
Coupling of protein motion to electron transfer: molecular dynamics and stochastic quantum mechanics study of photosynthetic reaction centers, K. Schulten and M. Tesch 158 (1991) 421
A molecular dynamics simulation of the C-terminal fragment of the L7/L12 ribosomal protein in solution, V. Daggett and M. Levitt 158 (1991) 501
Theoretical and experimental study on the electronic spectrum and photophysics of Michler's hydrol blue, I. Baraldi, A. Carnevali, F. Momicchioli and G. Ponterini 160 (1992) 85
The Pariser–Parr–Pople model for trans-polyenes. II. Parametrization and ground state dynamics, W. Förner 160 (1992) 189
Intramolecular charge transfer and trans–cis isomerization of the DCM styrene dye in polar solvents. A CS INDO MRCI study, S. Marguet, J.C. Mialocq, P. Millie, G. Berthier and F. Momicchioli 160 (1992) 265
Electronic spectra and transitions of the fullerene C_{60}, S. Leach, M. Vervloet, A. Desprès, E. Bréheret, J.P. Hare, T.J. Dennis, H.W. Kroto, R. Taylor and D.R.M. Walton 160 (1992) 451

–polymeric and biological

Picosecond time-resolved absorption and fluorescence in the bacteriorhodopsin photocycle: vibrationally-excited species, D. Blanchard, D.A. Gilmore, T.L. Brack, H. Lemaire, D. Hughes and G.H. Atkinson 154 (1991) 155
On the disordered distribution of defects in transpolyacetylene, F.C. Lavarda, D.A. dos Santos, D.S. Galvão and B. Laks 155 (1991) 1
Chiral discrimination: a model for the interaction between an helicoidal system and an amino acid molecule, E. Alvira, J. Breton, J. Plata and C. Girardet 155 (1991) 7
Shape resonances in photoionizations of cyanoacetylene. Experimental and theoretical investigations of the $\tilde{X}^2\Pi$, $\tilde{A}^2\Sigma$ and $\tilde{B}^2\Pi$ ionizations up to a photon energy of 28 eV, J. Kreile, H.-D. Kurland, W. Seibel and A. Schweig 155 (1991) 99
Monte Carlo and mean field studies of a polyelectrolyte in salt solution, C.E. Woodward and B. Jönsson 155 (1991) 207
Theoretical study of multiple-scattering effects in the X-ray absorption spectra of iron-porphyrins, F. Bohr and M.F. Ruiz-López 156 (1991) 55
Molecular dynamics simulation of superoxide interacting with superoxide dismutase, J. Shen and J.A. McCammon 158 (1991) 191
Comparison of lattice Monte Carlo dynamics and Brownian dynamics folding pathways of α-helical hairpins, A. Rey and J. Skolnick 158 (1991) 199
Molecular dynamics study of the photodissocation of carbon monoxide from myoglobin: ligand dynamics in the first 10 ps, J.E. Straub and M. Karplus 158 (1991) 221
Protein relaxation dynamics in human myoglobin, D.G. Lambright, S. Balasubramanian and S.G. Boxer 158 (1991) 249

Quantum simulation of conformation reorganization in the electron transfer reactions of tuna cytochrome c, C. Zheng, J.A. McCammon and P.G. Wolynes 158 (1991) 261
An NMR study of the backbone dynamics of staphylococcal nuclease in the crystalline state, H.B.R. Cole and D.A. Torchia 158 (1991) 271
Time- and temperature dependence of large-scale conformational transitions in myoglobin, R.D. Young, H. Frauenfelder, J.B. Johnson, D.C. Lamb, G.U. Nienhaus, R. Philipp and R. Scholl 158 (1991) 315
Evidence for proximal control of ligand specificity in hemeproteins: absorption and Raman studies of cryogenically trapped photoproducts of ligand bound myoglobins, A.M. Ahmed, B.F. Campbell, D. Caruso, M.R. Chance, M.D. Chavez, S.H. Courtney, J.M. Friedman, I.E.T. Iben, M.R. Ondrias and M. Yang 158 (1991) 329
Fluorescence and molecular dynamics study of the internal motion of the buried tryptophan in bacteriophage T4 lysozyme: effects of temperature and alteration of nonbonded networks, D.L. Harris and B.S. Hudson 158 (1991) 353
The effects of environment and hydration on protein dynamics: a simulation study of myoglobin, P.J. Steinbach, R.J. Loncharich and B.R. Brooks 158 (1991) 383
Theory of long time peptide dynamics: test of various reduced descriptions and role of internal variables, Y. Hu, G.R. Fleming, K.F. Freed and A. Perico 158 (1991) 395
The effects of solvent on the conformation and the collective motions of protein: normal mode analysis and molecular dynamics simulations of melittin in water and in vacuum, A. Kitao, F. Hirata and N. Gō 158 (1991) 447
Far-infrared perturbation of electron tunneling in reaction centers?, R.H. Austin, M.K. Hong, C. Moser and J. Plombon 158 (1991) 473
Dynamics of the hydrate and amide groups of crystalline ribonuclease and lysozyme, M.G. Usha, J. Speyer and R.J. Wittebort 158 (1991) 487
^{23}Na relaxation in DNA solutions. Influence of intercalation on correlation times and coupling constants, M. Hald and J.P. Jacobsen 159 (1992) 257
The Pariser–Parr–Pople model for trans-polyenes. II. Parametrization and ground state dynamics, W. Förner 160 (1992) 189
Computational experiments on the intramolecular energy flow in macromolecules, B.G. Sumpter and D.W. Noid 160 (1992) 393

Molecular aggregates

Time-dependent fluorescence depolarization arising from exciton annihilation in confined molecular domains, G. Juzeliūnas 151 (1991) 169
Emission of Xe:N(^{2}P) collision complexes near the N(^{2}P→^{2}D) lines, A.F. Vilesov, J. Wildt and E.H. Fink 153 (1991) 531
Pressure dependence of the polarized reflectance spectrum of a solid charge-transfer complex, perylene-hexacyanobutadiene (HCBD), T. Ida, K. Yakushi, H. Kuroda, H. Yamochi and G. Saito 156 (1991) 113
Test-particle model potentials for hydrogen-bonded complexes: complexes formed from HCN, HF, H_2O, NH_3, $HCONH_2$, $HCONHCH_3$, guanine and cytosine, K.P. Sagarik, V. Pongpituk, S. Chaiyapongs and P. Sisot 156 (1991) 439
Pressure dependence of the polarized reflectance spectrum of a solid charge-transfer complex, perylene-hexacyanobutadiene (HCBD), Chem. Phys. 156 (1991) 113–122. Erratum, T. Ida, K. Yakushi, H. Kuroda, H. Yamochi and G. Saito 157 (1991) 305
Single-crystal EPR and ^{15}N powder ENDOR studies of $[(C_4H_9)_4N][Tc^{VI}NBr_4/Tc^{V}OBr_4]$, K. Köhler, R. Kirmse, R. Böttcher and U. Abram 160 (1992) 281

UV photoemission spectroscopic studies on molecular aggregation of triphenylamines dispersed in polycarbonate thin films, N. Sato and M. Yoshikawa 160 (1992) 289

–dimers

Multiphoton dissociation dynamics of highly excited states of CS_2 and CS_2 clusters, E. Patsilinakou, D. Proch and C. Fotakis 153 (1991) 503

Ab initio study of the infrared photoconversion in the water–hydrogen iodide system, Y. Hannachi, B. Silvi, J.P. Perchard and Y. Bouteiller 154 (1991) 23

Rotational spectrum and structure of the linear HCN–HCCH dimer, A.I. Jaman, T.C. Germann, H.S. Gutowsky, J.D. Augspurger and C.E. Dykstra 154 (1991) 281

Core–valence correlation effects on some Cu clusters, H. Åkeby and L.G.M. Pettersson 155 (1991) 197

Fluorescence depolarization in nonlinear molecular pairs, D. Gülen 156 (1991) 123

Ab initio calculation of the second virial coefficient of neon and the potential energy curve of Ne_2, R. Eggenberger, S. Gerber, H. Huber and D. Searles 156 (1991) 395

A time-resolved fluorescence study of electronic excitation energy transport in concentrated dye solutions, A.D. Scully, A. Matsumoto and S. Hirayama 157 (1991) 253

On the fluorescence depolarization in bis-(N-carbazolyl) compounds, M. Hennecke and H.F. Kauffmann 157 (1991) 391

Driven damped harmonic oscillators perturbed by the parity operator, P. Blaise, M. Giry and O. Henri-Rousseau 159 (1992) 169

–van der Waals molecules

The submillimeter rotation-tunneling spectrum of Ar–D_2O and Ar–NH_3, E. Zwart and W.L. Meerts 151 (1991) 407

The trans-stilbene–Ar van der Waals complex. Vibrationally averaged substitution structure in its S_0 and S_1 electronic states, B.B. Champagne, D.F. Plusquellic, J.F. Pfanstiel, D.W. Pratt, W.M. van Herpen and W.L. Meerts 156 (1991) 251

A fluorescence characterization of the *p*-difluorobenzene–argon van der Waals complex. Energy levels, geometries and dissociation energies, M.-C. Su, H.-K. O and C.S. Parmenter 156 (1991) 261

A combining rule calculation of the van der Waals potentials of the rare-gas hydrides, K.T. Tang and J.P. Toennies 156 (1991) 413

–clusters

Theoretical study of the electronic states of BeLi and Be_2^+, I. Fischer, V.E. Bondybey, P. Rosmus and H.-J. Werner 151 (1991) 295

Model potentials in numerical local density functional methods, G.L. Gutsev, V.K. Gryaznov and V.A. Nasluzov 154 (1991) 291

An electrostatic-surface stability interpretation of the "hydrophobic" force inferred to occur between mica plates in solutions of soluble surfactants, R. Podgornik and V.A. Parsegian 154 (1991) 477

Core–valence correlation effects on some Cu clusters, H. Åkeby and L.G.M. Pettersson 155 (1991) 197

The structure of mixed watery clusters, B.R. Veenstra, H.C. Meijers, P.J. de Lange and J. Kommandeur 156 (1991) 157

Isomer-specific radiative lifetimes of molecular heteroclusters, D. Bahatt, U. Even, E. Shalev, N. Ben-Horin and J. Jortner 156 (1991) 223

Electronic spectra and proton transfer in the phenol/$(NH_3)_n$ clusters in argon matrices, C. Crépin and A. Tramer 156 (1991) 281

Many-body calculations of the core hole spectra of NiCO, M. Ohno and P. Decleva 156 (1991) 309
Nodal configurations and many-body energies in Li_3^{3+}, F_3^{3-}, $Li_2^{2+}F^-$ and $Li^+F_2^{2-}$ ions at crystal and cluster geometries, A.S. Shalabi 156 (1991) 359
Theoretical study of optical excitations of linear C_4^-, L. Adamowicz 156 (1991) 387
The structure and stability of Cl_n^- clusters, $n=2$–7, G.L. Gutsev 156 (1991) 427
From cluster to crystal: ab initio calculations of the OH^- frequency in lithium hydroxide monohydrate, K. Hermansson 159 (1992) 67
Nuclear quadrupole interaction of $^{99}Mo(\beta^-)^{99}Tc$ in various molybdenum sulfur cluster compounds and thermal decomposition products of $(NH_4)_2[Mo_3S(S_2)_6]\cdot nH_2O$ ($n=0$–2), P. Mottner, A. Lerf, T. Butz, H. Knözinger, A. Müller, V. Wittneben and E. Krickemeyer 160 (1992) 327
Many-body calculation of the XPS core hole spectra of NiN_2, P. Decleva and M. Ohno 160 (1992) 341
Many-body calculation of the core hole spectra of PdCO, P. Decleva and M. Ohno 160 (1992) 353

–complexes
A multisurface classical trajectory study of the dynamics of the reaction $O(^1D_2)+H_2\rightarrow OH(v', J', \Theta')+H$ using the diatomics in molecules method, P.J. Kuntz, B.I. Niefer and J.J. Sloan 151 (1991) 77
The H_2O_2–NO_2^- and $H_2NO_4^-$ isomers of the nitrate anion–water complex, M. Shen, Y. Xie, H.F. Schaefer III and C.A. Deakyne 151 (1991) 187
EPR investigation of chromium(III) complexes: analysis of their frozen solution and magnetically dilute powder spectra, R.P. Bonomo, A.J. Di Bilio and F. Riggi 151 (1991) 323
Anomalous magnetic effects. The role of association in the recombination of singlet radical pairs in liquids, N.V. Shokhirev, E.C. Korolenko, M.B. Taraban and T.V. Leshina 154 (1991) 237
Low-temperature chemical reactions. Effect of symmetrically coupled vibrations in collinear exchange reactions, V.A. Benderskii, V.I. Goldanskii and D.E. Makarov 154 (1991) 407
Circular dichroism spectrum of gadolinium diglycolate single crystal, T. Kundu, A.K. Banerjee and M. Chowdhury 156 (1991) 95
MO LCAO analysis of the vibronic instability of the $CuCl_5^{3-}$ trigonal bipyramidal configuration. Critical view on the angular overlap model in vibronic problems, V.Z. Polinger, N.N. Gorinchoi and I.B. Bersuker 159 (1992) 75
Collision-induced emission of $O_2(a\,^1\Delta_g\rightarrow X\,^3\Sigma_g^-)$ in the gas phase, J. Wildt, E.H. Fink, P. Biggs, R.P. Wayne and A.F. Vilesov 159 (1992) 127
A matrix isolation study of the water–formaldehyde complex. The far-infrared region, B. Nelander 159 (1992) 281
Single-crystal EPR and ^{15}N powder ENDOR studies of $[(C_4H_9)_4N][Tc^{VI}NBr_4/Tc^{V}OBr_4]$, K. Köhler, R. Kirmse, R. Böttcher and U. Abram 160 (1992) 281

Free radicals (including hydronium and muonium)
The diagmagnetic properties of the $\cdot NF_2$ radical by magic doublet rotational Zeeman spectroscopy, U.E. Frank and W. Hüttner 152 (1991) 261
Electron relaxation dynamics of Mu ALCR spectra, S.R. Kreitzman 152 (1991) 353
Theory of multiquantum optically detected ESR spectra of radical pairs. I. General theory. Resonances in parallel radio-frequency field, V.A. Morozov and A.B. Doktorov 153 (1991) 313
Theory of multiquantum optically detected ESR spectra of radical pairs. II. Resonances in perpendicular radio-frequency field, V.A. Morozov and A.B. Doktorov 153 (1991) 333
Anomalous magnetic effects. The role of association in the recombination of singlet radical pairs in liquids, N.V. Shokhirev, E.C. Korolenko, M.B. Taraban and T.V. Leshina 154 (1991) 237

Kinetics and magnetic field effect in geminate recombination of triplet radical pairs adsorbed onto porous glass studied by laser flash technique, P.P. Levin, I.V. Katalnikov and V.A. Kuzmin 154 (1991) 449
Intramolecular dynamics of the C_4H_8NH radical cation. An application of the anisotropic exchange theory for powder ESR lineshapes, L. Sjöqvist, N.P. Benetis, A. Lund and J. Maruani 156 (1991) 457
Excited states of hydrogen emitted from a graphite diffusion source: Arrhenius behaviour, E. Wallin and L. Holmlid 159 (1992) 313
Theory of geminate recombination of radical pairs with instantaneously changing spin Hamiltonian. I. General theory and kinematic approximation, A.B. Doktorov, S.A. Mikhailov and P.A. Purtov 160 (1992) 223
Theory of geminate recombination of radical pairs with instantaneously changing spin-Hamiltonian. II. Method of summation of re-encounter contributions, A.B. Doktorov, S.A. Mikhailov and P.A. Purtov 160 (1992) 239
Temperature dependence of cyanogen radical reactions with selected alkanes: CN reactivities towards primary, secondary and tertiary C–H bonds, D.L. Yang, T. Yu, N.S. Wang and M.C. Lin 160 (1992) 307
CN radical reactions with selected olefins in the temperature range 174–740 K, D.L. Yang, T. Yu, N.S. Wang and M.C. Lin 160 (1992) 317
The formulae for calculation of *g*-tensor shifts in third-order perturbation theory, E.N. Heifets 160 (1992) 363
Experimental and theoretical investigation of the reaction $CF_3+NO+M \rightarrow CF_3NO+M$ from 0.5 to 12 Torr and from 253 to 373 K, J. Masanet, F. Caralp, L. Ley and R. Lesclaux 160 (1992) 383
The structure and dynamics of 1,3,5-cycloheptatriene and 1,3-cycloheptadiene radical cations in low temperature matrices. An ESR investigation, Y. Kubozono, T. Miyamoto, M. Aoyagi, M. Ata, Y. Matsuda, Y. Gondo, H. Nakamura and T. Matsuo 160 (1992) 421

Quasiparticles (including excitons)

Time-dependent fluorescence depolarization arising from exciton annihilation in confined molecular domains, G. Juzeliūnas 151 (1991) 169
The solvated electron in an electrolyte solution, V.D. Lakhno and O.V. Vasil'ev 153 (1991) 147
Laser excitation and resolved emission spectra of supersonically cooled aluminum dimer, M.F. Cai, C.C. Carter, T.A. Miller and V.E. Bondybey 155 (1991) 233
A cluster model of the charge transfer interaction between an impurity and the host molecular crystal, P. Petelenz and A. Eilmes 155 (1991) 247
Fluorescence depolarization in nonlinear molecular pairs, D. Gülen 156 (1991) 123
Two-dimensional model of charge transfer excitons in polyacene crystals, P. Petelenz and M. Slawik 157 (1991) 169
The treatment of electron correlation in aperiodic systems. IV. Exciton bands and double ionization potentials, C.-M. Liegener 157 (1991) 183

Defects and impurities

Fluorescence detected level-anticrossing and spin coherence of a localized triplet state in diamond, E. van Oort and M. Glasbeek 152 (1991) 365
Kinetics of the reactions of intrinsic and phosphorus doped polycrystalline silicon with molecular chlorine, Z.H. Walker and E.A. Ogryzlo 153 (1991) 483

A theoretical investigation of the hyperfine properties of normal and anomalous muonium in elemental semiconductors: diamond, silicon and germanium, M. Casarin, G. Granozzi, E. Tondello and A. Vittadini 154 (1991) 385
Laser excitation and resolved emission spectra of supersonically cooled aluminum dimer, M.F. Cai, C.C. Carter, T.A. Miller and V.E. Bondybey 155 (1991) 233
A cluster model of the charge transfer interaction between an impurity and the host molecular crystal, P. Petelenz and A. Eilmes 155 (1991) 247
Electron transfer induced by liquid defect motion. Exact solution, D.V. Matyushov 155 (1991) 331
New Monte Carlo simulations of many-particle stochastic dynamics: growth of correlations and local self-ordering during annihilation of like particles, R. Brown and N.A. Efremov 155 (1991) 357
Site effects in spectra of matrix-isolated diatomic molecules: a modelling approach, M. Winter, K. Seranski and U. Schurath 159 (1992) 235
Site-resolved vibronic spectra of matrix-isolated NBr: comparison with model calculations, K. Seranski, M. Winter and U. Schurath 159 (1992) 247
The formulae for calculation of *g*-tensor shifts in third-order perturbation theory, E.N. Heifets 160 (1992) 363

Ions and charge carriers

The H_2O_2–NO_2^- and $H_2NO_4^-$ isomers of the nitrate anion–water complex, M. Shen, Y. Xie, H.F. Schaefer III and C.A. Deakyne 151 (1991) 187
Hydroxonium ion formation in collisions of $H_2O^+ + D_2O$ and $D_2O^+ + H_2O$: a crossed-beam scattering study, J. Vančura and Z. Herman 151 (1991) 249
The probability of non-adiabatic electron transfer as a function of friction, A.I. Burshtein and A.A. Zharikov 152 (1991) 23
Chemical reaction rates and solvation dynamics in electrolyte solutions: ion atmosphere friction, G. van der Zwan and J.T. Hynes 152 (1991) 169
Heavy ions in mixtures of light gases: Fokker–Planck equation and its solution, L. Ferrari 153 (1991) 115
Xerographic dark discharge of PVK:TNF photoconductive material, J.-Y. Moisan, B. André and R. Lever 153 (1991) 305
Generalized Einstein relations for ions in molecular gases, A.D. Koutselos and E.A. Mason 153 (1991) 351
Model calculations of the anthracene photocurrent spectrum, P. Petelenz and D. Mucha 154 (1991) 145
Potential curves and predissociation rates for the heavy species HBr^{2+} and DBr^{2+}, A. Banichevich, S.D. Peyerimhoff, B.A. Hess and M.C. van Hemert 154 (1991) 199
On the solution of the Debye–Smoluchowski equation with a Coulomb potential. III. The case of a Boltzmann initial distribution and a perfectly absorbing sink, S.D. Traytak 154 (1991) 263
Potential of mean force by constrained molecular dynamics: a sodium chloride ion-pair in water, E. Guàrdia, R. Rey and J.A. Padró 155 (1991) 187
Localization and correlation corrections in electronic interactions through single bonded hydrocarbon spacers, M. Braga, A. Broo and S. Larsson 156 (1991) 1
Theoretical study of optical excitations of linear C_4^-, L. Adamowicz 156 (1991) 387
Interaction potentials in rare gas–halide ion systems, V. Kellö and A.J. Sadlej 157 (1991) 123
The benzene dication: energies of excited states determined by double-charge-transfer spectroscopy using OH^+ and F^+ projectile ions, W.J. Griffiths and F.M. Harris 157 (1991) 299
Quantum-chemical calculations of the hydration energies of organic cations and anions in the framework of a continuum solvent approximation, G.E. Chudinov, D.V. Napolov and M.V. Basilevsky 160 (1992) 41

Laser-initiated chain reactions and microexplosions in solid solutions of methylcyclopropane and chlorine, Chem. Phys. 156 (1991) 141–148. Erratum, T.J. Tague Jr. and C.A. Wright 157 (1991) 305

Phenomena

Molecular structure

Ab initio SCF study on $LiClO_4$ and Li_2SO_4 molecules: geometries and vibrational frequencies, F. Ramondo, L. Bencivenni, R. Caminiti and C. Sadun 151 (1991) 179
The H_2O_2–NO_2^- and $H_2NO_4^-$ isomers of the nitrate anion–water complex, M. Shen, Y. Xie, H.F. Schaefer III and C.A. Deakyne 151 (1991) 187
Jahn–Teller effect and dissociation from the ground state of CF_4^+, J.M. García de la Vega and E. San Fabián 151 (1991) 335
The submillimeter rotation-tunneling spectrum of Ar–D_2O and Ar–NH_3, E. Zwart and W.L. Meerts 151 (1991) 407
Avoided-crossing molecular-beam study of the torsion–rotation energy levels of CH_3CF_3, W.L. Meerts and I. Ozier 152 (1991) 241
Observable-dedicated molecular orbitals. I. Method and illustrations, J. Miralles, R. Caballol and J.-P. Malrieu 153 (1991) 25
The structures and stability of the $Si_3H_6^{2+}$ dications. A theoretical study, T. Kudo and S. Nagase 153 (1991) 379
Bond formation between positively charged species. Non-adiabatic analysis and valence-bond model in the CO^{2+} case, N. Levasseur, Ph. Millie, P. Archirel and B. Levy 153 (1991) 387
Theoretical study of the reaction of OH with HNO, M.R. Soto, M. Page and M.L. McKee 153 (1991) 415
Ab initio study of the infrared photoconversion in the water–hydrogen iodide system, Y. Hannachi, B. Silvi, J.P. Perchard and Y. Bouteiller 154 (1991) 23
Isomerization and unimolecular rearrangement channels of dithioformic acid, Y. Tao 154 (1991) 221
A theoretical study on the internal rotation and hyperfine structures of the ethyl radical (CH_3–CH_2), H.U. Suter and T.K. Ha 154 (1991) 227
The generator coordinate Hartree–Fock method for molecular systems. Formalism and first applications to H_2, LiH and Li_2, H.F.M. da Costa, A.B.F. da Silva, J.R. Mohallem, A.M. Simas and M. Trsic 154 (1991) 379
On the disordered distribution of defects in transpolyacetylene, F.C. Lavarda, D.A. dos Santos, D.S. Galvão and B. Laks 155 (1991) 1
On the BiF bond dissociation energy and an evaluation of the BiF red emission band systems, T.C. Devore, L. Brock, R. Kahlscheuer, K. Dulaney and J.L. Gole 155 (1991) 423
^{14}N NQR investigation of some thermochromic and photochromic salicylideneanilines and related compounds, E. Hadjoudis, F. Milia, J. Seliger, V. Zagar and R. Blinc 156 (1991) 149
On the BiF bond dissociation energy and an evaluation of the BiF red emission band systems, Chem. Phys. 155 (1991) 423–433. Erratum, T. Devore, L. Brock, R. Kahlscheuer, K. Dulaney and J.L. Gole 156 (1991) 156
The trans-stilbene–Ar van der Waals complex. Vibrationally averaged substitution structure in its S_0 and S_1 electronic states, B.B. Champagne, D.F. Plusquellic, J.F. Pfanstiel, D.W. Pratt, W.M. van Herpen and W.L. Meerts 156 (1991) 251
A fluorescence characterization of the *p*-difluorobenzene–argon van der Waals complex. Energy levels, geometries and dissociation energies, M.-C. Su, H.-K. O and C.S. Parmenter 156 (1991) 261
Nodal configurations and many-body energies in Li_3^{3+}, F_3^{3-}, $Li_2^{2+}F^-$ and $Li^+F_2^{2-}$ ions at crystal and cluster geometries, A.S. Shalabi 156 (1991) 359

Test-particle model potentials for hydrogen-bonded complexes: complexes formed from HCN, HF, H_2O, NH_3, $HCONH_2$, $HCONHCH_3$, guanine and cytosine, K.P. Sagarik, V. Pongpituk, S. Chaiyapongs and P. Sisot 156 (1991) 439
The electronic states of the azines. V. Pyridazine, studied by VUV absorption, near threshold electron energy-loss spectroscopy and ab initio multi-reference configuration interaction calculations, M.H. Palmer and I.C. Walker 157 (1991) 187
Ring-puckering and internal rotation barriers in N,N′-dimethylethyleneurea, J.C. Otero, J.I. Marcos, E. López-Cantarero and A. Chacón 157 (1991) 201
The structure and stability of S_2F_{10} and S_2F_{11} and their anions, G.L. Gutsev 158 (1991) 33
Ab initio study on the coordination structures of $M^+XY_3^-$ and $M^+XY_4^-$ ion pairs, F. Ramondo, L. Bencivenni and V. Di Martino 158 (1991) 41
Evidence for proximal control of ligand specificity in hemeproteins: absorption and Raman studies of cryogenically trapped photoproducts of ligand bound myoglobins, A.M. Ahmed, B.F. Campbell, D. Caruso, M.R. Chance, M.D. Chavez, S.H. Courtney, J.M. Friedman, I.E.T. Iben, M.R. Ondrias and M. Yang 158 (1991) 329
Coupling of protein motion to electron transfer: molecular dynamics and stochastic quantum mechanics study of photosynthetic reaction centers, K. Schulten and M. Tesch 158 (1991) 421
The effects of solvent on the conformation and the collective motions of protein: normal mode analysis and molecular dynamics simulations of melittin in water and in vacuum, A. Kitao, F. Hirata and N. Gō 158 (1991) 447
Dynamics of the hydrate and amide groups of crystalline ribonuclease and lysozyme, M.G. Usha, J. Speyer and R.J. Wittebort 158 (1991) 487
MO LCAO analysis of the vibronic instability of the $CuCl_5^{3-}$ trigonal bipyramidal configuration. Critical view on the angular overlap model in vibronic problems, V.Z. Polinger, N.N. Gorinchoi and I.B. Bersuker 159 (1992) 75
Variational approach to continuum orbitals in a spline basis: an application to H_2^+ photoionization, M. Brosolo and P. Decleva 159 (1992) 185
Comparative study on the structures and energies of the SiX_3, GeX_3 and SnX_3 series of radicals (X=H, F, Cl), J. Moc, J.M. Rudziński and H. Ratajczak 159 (1992) 197
A theoretical investigation of the electronic structure, hyperfine properties and binding energies of muonium centres in cuprous chloride, M. Casarin, G. Granozzi, E. Tondello and A. Vittadini 159 (1992) 365
Principal-component self-modeling analysis of fluorescence for some trans-diarylethylenes. A comparison with kinetic analysis, A. Spalletti, G. Bartocci, F. Masetti, U. Mazzucato and G. Cruciani 160 (1992) 131
The Pariser–Parr–Pople model for trans-polyenes. I. Ab initio and semiempirical study of the bond alternation in trans-butadiene, W. Förner 160 (1992) 173
Evidence for a gauche minor-conformer of 1,3-butadiene, R. Engeln, D. Consalvo and J. Reuss 160 (1992) 427

Vibrations and rotations of molecules

Calculation of the vibrational frequency and line strength versus applied field of carbon monoxide, J.L. Andrés, M. Duran, A. Lledós and J. Bertrán 151 (1991) 37
Rotation–vibration energies of FHF^- and $ClHCl^-$ from high-level correlated calculations of potential energy surfaces, V. Špirko, A. Čejchan and G.H.F. Diercksen 151 (1991) 45
A classical study on the vibrational motion of a diatomic molecule in a collisional vibronic excitation, R.F.M. Lobo and A.M.C. Moutinho 151 (1991) 95

Time-resolved relaxation of one- and two-vibron states in the rubidium perchlorate crystal, G.M. Gale and P. Schanne 151 (1991) 127
Theoretical infrared spectra of large carbon clusters, D. Bakowies and W. Thiel 151 (1991) 309
Solvent cage effects and chemical dynamics in liquids, F. Patron and S.A. Adelman 152 (1991) 121
The diagmagnetic properties of the $\cdot NF_2$ radical by magic doublet rotational Zeeman spectroscopy, U.E. Frank and W. Hüttner 152 (1991) 261
FIR LMR spectra of FO_2: some classic examples of level anticrossing resonances, U. Bley, P.B. Davies, M. Grantz, T.J. Sears and F. Temps 152 (1991) 281
Mixing of the vibrational angular momentum components of multiply degenerate vibronic states of benzene by vibrational *l*-type resonance, E. Riedle and J. Pliva 152 (1991) 375
The influence of the spin–orbit and the hyperfine interaction on the asymptotic behaviour of the $A\,^1\Sigma_u^+$ state of Na_2, H. Knöckel, T. Johr, H. Richter and E. Tiemann 152 (1991) 399
Vibrational structure of the solvated glycine zwitterion, J.S. Alper, H. Dothe and D.F. Coker 153 (1991) 51
Relaxation cross sections for transfer of rotational angular momentum in a semiclassical approximation, A.V. Storozhev and M.L. Strekalov 153 (1991) 99
The magnetizability and *g*-factor surfaces of ammonia, S.P.A. Sauer, V. Špirko and J. Oddershede 153 (1991) 189
Highly excited states of nitric oxide studied by high-resolution resonance-enhanced multiphoton ionization spectroscopy, Y. Luo, Y.D. Cheng, H. Ågren, R. Maripuu, W. Seibt, L. Öhlund, P. Ejeklint, B. Carman, K.Z. Xing, Y. Achiba and K. Siegbahn 153 (1991) 473
Periodic orbits and quantum localization in the van der Waals systems CO–Ar, L. Zachilas and S.C. Farantos 154 (1991) 55
Connecting level statistics and reaction dynamics: mode selective decay of resonant states for HXXH-type molecules, B. Hartke and W. Karrlein 154 (1991) 63
Lattice dynamics of the orthorhombic phase of $KClO_4$: Ewald's method in molecular coordinates, G.F. Signorini, R. Righini and V. Schettino 154 (1991) 245
Quantum kinetic energy operator for a group of particles in terms of scalar basic rotational invariant coordinates derived from a generalized Jacobi vector (GJV) description. III. A metric tensors approach, J.P. Leroy, H. Rabitz and R. Wallace 154 (1991) 395
Triplet state IR spectroscopy of aromatic homocycles and heterocycles, H. Krumschmidt and C. Kryschi 154 (1991) 459
Effects of homogeneous and inhomogeneous broadening mechanisms and molecular rearrangement dynamics on frequency resolved and time resolved coherent Raman intensities, H. Okamoto 155 (1991) 291
A vibrational study of the CD_3H molecule in the curvilinear formulation, C. Iung and C. Leforestier 155 (1991) 369
The vibrational spectra of the monohalogenated cyclopropanes: ab initio calculations and an experimental study of fluorocyclopropane, C. Kaupert, H. Heydtmann and W. Thiel 156 (1991) 85
Methyl torsion in $C_2H_{4-n}(CH_3)_n$, $n=1$ or 2, R. Engeln and J. Reuss 156 (1991) 215
A fluorescence characterization of the *p*-difluorobenzene–argon van der Waals complex. Energy levels, geometries and dissociation energies, M.-C. Su, H.-K. O and C.S. Parmenter 156 (1991) 261
Nuclear quadrupole coupling constants of rovibrational levels of all isotopic species of BH^+ in their $X\,^2\Sigma^+$ and $B'\,^2\Sigma^+$ states, J. Vojtík, L. Češpiva, I. Paidarová and J. Šavrda 156 (1991) 369
Construction of bound-state potential energy curves of diatomic molecules from spectroscopic data, C.G. Diaz, F.M. Fernández and E.A. Castro 157 (1991) 35
Adiabatic calculations and properties of the He_2^+ molecular ion, J. Ackermann and H. Hogreve 157 (1991) 75

Molecular dynamics study of the photodissocation of carbon monoxide from myoglobin: ligand dynamics in the first 10 ps, J.E. Straub and M. Karplus 158 (1991) 221
Far-infrared perturbation of electron tunneling in reaction centers?, R.H. Austin, M.K. Hong, C. Moser and J. Plombon 158 (1991) 473
Interference and Fermi-resonant two-vibron bound states, P. Schanne and G.M. Gale 159 (1992) 1
Ab initio calculation of anharmonic force fields for the methyl, silyl, germyl, and stannyl halides, W. Schneider and W. Thiel 159 (1992) 49
From cluster to crystal: ab initio calculations of the OH^- frequency in lithium hydroxide monohydrate, K. Hermansson 159 (1992) 67
Quasiclassical trajectory study of the effect of reactant rotation on the reaction $B^+ + HD \rightarrow BH^+(BD^+) + D(H)$, V. Klimo, J. Urban and J. Tiňo 159 (1992) 141
A matrix isolation study of the water–formaldehyde complex. The far-infrared region, B. Nelander 159 (1992) 281
The importance of periodic orbits in analysing photodissociation resonances: the O_3 case, S.C. Farantos 159 (1992) 329
A weak-mode representation of floppy molecules. I. Potential energy, C. Saint-Espès, X. Chapuisat and F. Schneider 159 (1992) 377
A weak-mode representation of floppy molecules. II. Kinetic energy and total Hamiltonian matrix, X. Chapuisat and C. Saint-Espès 159 (1992) 391
Methyl tunnelling in solid diacetyl, A.M. Alsanoosi and A.J. Horsewill 160 (1992) 25
Computational experiments on the intramolecular energy flow in macromolecules, B.G. Sumpter and D.W. Noid 160 (1992) 393

Electronic structure and states

Theoretical study of the spectroscopy of Al_2^+, M. Rosi, C.W. Bauschlicher Jr. and S.R. Langhoff 151 (1991) 1
Electronic structure of linear form of OCuO, Y. Mochizuki, K. Tanaka and H. Kashiwagi 151 (1991) 11
Ab initio molecular orbital treatment of hydroxylamine–X^+–water and hydroxylamine–X^+–ammonia (X=H, Li) clusters, M. Alcamí, O. Mó and M. Yáñez 151 (1991) 21
The electronically excited states of 2-phenylindole, B. Albinsson, S. Eriksson, R. Lyng and M. Kubista 151 (1991) 149
Estimation of electronic correlation energies and binding energies for molecules composed of first-row atoms, K. Rościszewski, M. Chaumet and P. Fulde 151 (1991) 159
Quenching and rotational transfer rates in the $v'=0$ manifold of $OH(A^2\Sigma^+)$, J. Burris, J. Butler, T. McGee and W. Heaps 151 (1991) 233
Picosecond photodissociation and geminate radical recombination in alkane solutions of tetraphenylhydrazine, M.G. Hyde and G.S. Beddard 151 (1991) 239
Theoretical study of the electronic states of BeLi and Be_2^+, I. Fischer, V.E. Bondybey, P. Rosmus and H.-J. Werner 151 (1991) 295
Jahn–Teller effect and dissociation from the ground state of CF_4^+, J.M. García de la Vega and E. San Fabián 151 (1991) 335
Picosecond Stokes shift studies of solvent friction: experimental measurements of time-dependent band shape and integrated intensity, J.D. Simon and S.-G. Su 152 (1991) 143
Observation of level crossing and level anticrossing signals in the CO_2 laser Stark spectrum of POF_3 and their proposed application to electric field standards in laser Stark spectroscopy, K. Tanaka, K. Someya and T. Tanaka 152 (1991) 229
Theoretical study of the spectroscopy of the alkali oxides LiO, NaO, and KO, S.R. Langhoff, H. Partridge and C.W. Bauschlicher Jr. 153 (1991) 1

Ab initio calculations on the one- and two-photon electronic transitions of cyclopentadiene, spirononateraene, 1,4-cyclo-hexadiene, Dewar benzene, norbornadiene, and barrelene, V. Galasso 153 (1991) 13
The solvated electron in an electrolyte solution, V.D. Lakhno and O.V. Vasil'ev 153 (1991) 147
The electronic states of the azines. IV. Pyrazine, studied by VUV absorption, near-threshold electron energy-loss spectroscopy and ab initio multi-reference configuration interaction calculations, I.C. Walker and M.H. Palmer 153 (1991) 169
Estimation of the integral cross section for dissociative excitation of F_2 by electron impact, D.C. Cartwright, P.J. Hay and S. Trajmar 153 (1991) 219
Ferromagnetism of charge-transfer crystals, A.L. Tchougreeff and I.A. Misurkin 153 (1991) 371
The structures and stability of the $Si_3H_6^{2+}$ dications. A theoretical study, T. Kudo and S. Nagase 153 (1991) 379
Bond formation between positively charged species. Non-adiabatic analysis and valence-bond model in the CO^{2+} case, N. Levasseur, Ph. Millie, P. Archirel and B. Levy 153 (1991) 387
Heteronuclear transition metal diatomics: the bonding and electronic structure of ScNi, YNi, ScPd and YPd, K. Faegri Jr. and C.W. Bauschlicher Jr. 153 (1991) 399
Theoretical study of the reaction of OH with HNO, M.R. Soto, M. Page and M.L. McKee 153 (1991) 415
Emission of Xe:N(^{2}P) collision complexes near the N(^{2}P→^{2}D) lines, A.F. Vilesov, J. Wildt and E.H. Fink 153 (1991) 531
Calculation of excitation energies using quasidegenerate variational perturbation theory and multireference-averaged coupled-pair functional theory, M.A. Anderson and R.J. Cave 154 (1991) 1
Theoretical study of the electronic spectrum of ammonia: generalized oscillator strength calculations for the A–X transition, L. Chantranupong, G. Hirsch, R.J. Buenker, M. Kimura and M.A. Dillon 154 (1991) 13
An experimental and theoretical study of SF^{q+} (q=1–3) ions, K. Nagesha, V.R. Marathe and D. Mathur 154 (1991) 125
Model calculations of the anthracene photocurrent spectrum, P. Petelenz and D. Mucha 154 (1991) 145
Unusual features in the polarised single crystal electronic spectrum of $(NH_4)_2[V(H_2O)_6](SO_4)_2$: analysis of Fano antiresonance structure and bonding in the $[V(H_2O)_6]^{2+}$ complex, R.G. McDonald, R. Stranger, M.A. Hitchman and P.W. Smith 154 (1991) 179
Potential curves and predissociation rates for the heavy species HBr^{2+} and DBr^{2+}, A. Banichevich, S.D. Peyerimhoff, B.A. Hess and M.C. van Hemert 154 (1991) 199
Calculation of the inner shell excitation spectra and estimation of the electron scattering and dissociative attachment resonance energies of SF_6, SO_2, SF_2O, SF_2O_2, SF_4, SF_4O and S_2F_{10}, J.A. Tossell 154 (1991) 211
A theoretical study on the internal rotation and hyperfine structures of the ethyl radical (CH_3–CH_2), H.U. Suter and T.K. Ha 154 (1991) 227
Model potentials in numerical local density functional methods, G.L. Gutsev, V.K. Gryaznov and V.A. Nasluzov 154 (1991) 291
Absolute partial photoionization cross sections of ethylene, F.A. Grimm, T.A. Whitley, P.R. Keller and J.W. Taylor 154 (1991) 303
Oxygen K-shell excitation spectroscopy of hydrogen peroxide, E. Rühl and A.P. Hitchcock 154 (1991) 323
The generator coordinate Hartree–Fock method for molecular systems. Formalism and first applications to H_2, LiH and Li_2, H.F.M. da Costa, A.B.F. da Silva, J.R. Mohallem, A.M. Simas and M. Trsic 154 (1991) 379

A theoretical investigation of the hyperfine properties of normal and anomalous muonium in elemental semiconductors: diamond, silicon and germanium, M. Casarin, G. Granozzi, E. Tondello and A. Vittadini 154 (1991) 385
Energy levels of Cr^{3+} ions in C_{3i} sites of $Y_3Al_5O_{12}$, C.A. Morrison, J.B. Gruber and M.E. Hills 154 (1991) 437
On the disordered distribution of defects in transpolyacetylene, F.C. Lavarda, D.A. dos Santos, D.S. Galvão and B. Laks 155 (1991) 1
The first ionization potentials of some MH_{k+1}^- and $M_2H_{2k+1}^-$ anions calculated by a Green's function method, A.I. Boldyrev and W. von Niessen 155 (1991) 71
Semiempirical electrostatic polarization model of the ionic bonding in alkali and alkaline earth hydroxides and halides, J.M. Mestdagh and J.P. Visticot 155 (1991) 79
The optical spectrum of $Ba_2Zn[Cu]F_6$, D. Reinen, G. Steffen, M.A. Hitchman, H. Stratemeier, L. Dubicki, E.R. Krausz, M.J. Riley, H.E. Mathies, K. Recker and F. Wallrafen 155 (1991) 117
Lowest energy triplet states of group Vb hydrides: NH_3 (ND_3) and PH_3, M. Ben Arfa and M. Tronc 155 (1991) 143
Symmetry and vibronic coupling: the stereochemistry and the ground state potential surface of Cu^{2+} in five-coordination, D. Reinen and M. Atanasov 155 (1991) 157
Laser excitation and resolved emission spectra of supersonically cooled aluminum dimer, M.F. Cai, C.C. Carter, T.A. Miller and V.E. Bondybey 155 (1991) 233
Pulsed discharge source of supersonically cooled transient species, R. Schlachta, G. Lask, S.H. Tsay and V.E. Bondybey 155 (1991) 267
Effects of homogeneous and inhomogeneous broadening mechanisms and molecular rearrangement dynamics on frequency resolved and time resolved coherent Raman intensities, H. Okamoto 155 (1991) 291
Valence-shell electron momentum distributions of cyclopropane by symmetric noncoplanar (e,2e) spectroscopy, M.P. Banjavčić, T.A. Daniels and K.T. Leung 155 (1991) 309
On the BiF bond dissociation energy and an evaluation of the BiF red emission band systems, T.C. Devore, L. Brock, R. Kahlscheuer, K. Dulaney and J.L. Gole 155 (1991) 423
Photodissociation of CF_3I at 248 nm: kinetic energy dependence of the recoil anisotropy, P. Felder 155 (1991) 435
Circular dichroism spectrum of gadolinium diglycolate single crystal, T. Kundu, A.K. Banerjee and M. Chowdhury 156 (1991) 95
Electronic spectra of 4-nitro-pyridine-*n*-oxide (NPO) single crystals, M. Pierre, P.L. Baldeck, D. Block, R. Georges, H.P. Trommsdorff and J. Zyss 156 (1991) 103
Pressure dependence of the polarized reflectance spectrum of a solid charge-transfer complex, perylene-hexacyanobutadiene (HCBD), T. Ida, K. Yakushi, H. Kuroda, H. Yamochi and G. Saito 156 (1991) 113
Shape resonances in low-energy electron transmission and sulfur K-shell photoabsorption spectroscopies: CH_3SH, C_2H_5SH, $(CH_3)_2S$, $(C_2H_5)_2S$, C_6H_5SH, $C_6H_5SCH_3$, CH_3SCN, CH_3NCS, SCl_2, C. Dezarnaud, M. Tronc and A. Modelli 156 (1991) 129
^{14}N NQR investigation of some thermochromic and photochromic salicylideneanilines and related compounds, E. Hadjoudis, F. Milia, J. Seliger, V. Zagar and R. Blinc 156 (1991) 149
On the BiF bond dissociation energy and an evaluation of the BiF red emission band systems, Chem. Phys. 155 (1991) 423–433. Erratum, T. Devore, L. Brock, R. Kahlscheuer, K. Dulaney and J.L. Gole 156 (1991) 156
Magnetic field dependence of rotationally resolved excitation spectra of the $^1B_{3u}$ 0_0^0 transition of jet-cooled pyrazine, P.J. de Lange, H.Th. Jonkman and K.E. Drabe 156 (1991) 209

Many-body calculations of the core hole spectra of NiCO, M. Ohno and P. Decleva 156 (1991) 309
Nuclear quadrupole coupling constants of rovibrational levels of all isotopic species of BH^+ in their $X\,^2\Sigma^+$ and $B'\,^2\Sigma^+$ states, J. Vojtík, L. Češpiva, I. Paidarová and J. Šavrda 156 (1991) 369
The structure and stability of Cl_n^- clusters, $n=2$–7, G.L. Gutsev 156 (1991) 427
Laser excitation of the $A\,^3\Sigma_u^+$, $A'\,^3\Delta_u$ and $c\,^1\Sigma_u^-$ states of molecular oxygen, J. Wildt, G. Bednarek, E.H. Fink and R.P. Wayne 156 (1991) 497
Adiabatic calculations and properties of the He_2^+ molecular ion, J. Ackermann and H. Hogreve 157 (1991) 75
Singlet–triplet energy component differences in homonuclear diatomics: a multi-reference configuration interaction study of Hund's rule, K.V. Darvesh, P.D. Fricker and R.J. Boyd 157 (1991) 99
Transition probabilities for the $B\,^1\Delta_g$–$A\,^1\Pi_u$ and $B'\,^1\Sigma_g^+$–$A\,^1\Pi_u$ infrared bands of C_2. An ab initio study, P.J. Bruna and J.S. Wright 157 (1991) 111
Two-dimensional model of charge transfer excitons in polyacene crystals, P. Petelenz and M. Slawik 157 (1991) 169
The treatment of electron correlation in aperiodic systems. IV. Exciton bands and double ionization potentials, C.-M. Liegener 157 (1991) 183
Fluorescence analysis of two new TICT systems: 10-cyano-9,9′-bianthryl (CBA) and 10,10′-dicyano-9,9′-bianthryl (DCBA), S. Müller and J. Heinze 157 (1991) 231
Many-body calculation of the valence photoemission spectrum of ferrocene, M. Ohno, W. von Niessen and J. Schüle 158 (1991) 1
Radiative and radiationless depopulation of the excited intramolecular charge transfer states: aryl derivatives of aromatic amines, J. Herbich and A. Kapturkiewicz 158 (1991) 143
Satellite lines at the ionization threshold in charge transfer systems, W. Wardermann and W. von Niessen 159 (1992) 11
Site-resolved vibronic spectra of matrix-isolated NBr: comparison with model calculations, K. Seranski, M. Winter and U. Schurath 159 (1992) 247
Valence-shell electron momentum distributions and ionization energy spectra of tetramethylsilane by symmetric noncoplanar (e, 2e) spectroscopy, T. Daniels, H. Zhu, M.P. Banjavčić and K.T. Leung 159 (1992) 289
Assessment of Gaussian-weighted angular resolution functions in the comparison of quantum-mechanically calculated electron momentum distributions with experiment, P. Duffy, M.E. Casida, C.E. Brion and D.P. Chong 159 (1992) 347
A theoretical investigation of the electronic structure, hyperfine properties and binding energies of muonium centres in cuprous chloride, M. Casarin, G. Granozzi, E. Tondello and A. Vittadini 159 (1992) 365
Ab-initio multiple reference double-excitation configuration-interaction ground and excited state potential curves for the H_2N–NO_2 decomposition in nitramine, S. Roszak and J.J. Kaufman 160 (1992) 1
Electronic spectra of the naphthyridines: 2,7-naphthyridine, P. Wormell and A.R. Lacey 160 (1992) 55
Theoretical and experimental study on the electronic spectrum and photophysics of Michler's hydrol blue, I. Baraldi, A. Carnevali, F. Momicchioli and G. Ponterini 160 (1992) 85
The dissociation dynamics of low lying triplet states in butane and butene molecules, J.H.M. Beijersbergen, C.G. de Koster, W.J. van der Zande, P.G. Kistemaker and J. Los 160 (1992) 151
The Pariser–Parr–Pople model for trans-polyenes. I. Ab initio and semiempirical study of the bond alternation in trans-butadiene, W. Förner 160 (1992) 173
Intramolecular charge transfer and trans–cis isomerization of the DCM styrene dye in polar solvents. A CS INDO MRCI study, S. Marguet, J.C. Mialocq, P. Millie, G. Berthier and F. Momicchioli 160 (1992) 265

Single-crystal EPR and ^{15}N powder ENDOR studies of $[(C_4H_9)_4N][Tc^{VI}NBr_4/Tc^{V}OBr_4]$, K. Köhler, R. Kirmse, R. Böttcher and U. Abram 160 (1992) 281
The electronic structure of poly(*p*-phenylene vinylene), N. Sato, M. Lögdlund, R. Lazzaroni, W.R. Salaneck, J.-L. Brédas, D.D.C. Bradley, R.H. Friend and K.E. Ziemelis 160 (1992) 299
Many-body calculation of the XPS core hole spectra of NiN_2, P. Decleva and M. Ohno 160 (1992) 341
Many-body calculation of the core hole spectra of PdCO, P. Decleva and M. Ohno 160 (1992) 353
Electronic spectra and transitions of the fullerene C_{60}, S. Leach, M. Vervloet, A. Desprès, E. Bréheret, J.P. Hare, T.J. Dennis, H.W. Kroto, R. Taylor and D.R.M. Walton 160 (1992) 451
Pressure dependence of the polarized reflectance spectrum of a solid charge-transfer complex, perylene-hexacyanobutadiene (HCBD), Chem. Phys. 156 (1991) 113–122. Erratum, T. Ida, K. Yakushi, H. Kuroda, H. Yamochi and G. Saito 157 (1991) 305

Electric and magnetic properties

Calculation of the vibrational frequency and line strength versus applied field of carbon monoxide, J.L. Andrés, M. Duran, A. Lledós and J. Bertrán 151 (1991) 37
Symmetry and magnetic vibrational circular dichroism spectra of a doubly degenerate vibration and its combinations with non-degenerate vibrational modes, M. Pawlikowski and O. Sonnich Mortensen 151 (1991) 73
Triplet electron–proton cross-polarization by satisfying a modified Hartmann–Hahn condition, R.H. Fritsch, H. Brunner and K.H. Hausser 151 (1991) 261
The diagmagnetic properties of the $\cdot NF_2$ radical by magic doublet rotational Zeeman spectroscopy, U.E. Frank and W. Hüttner 152 (1991) 261
Anomalous structure in the $A^6\Sigma^+$–$X^6\Sigma^+$ transition of MnO caused by interference between two internal hyperfine perturbations, A.G. Adam, Y. Azuma, H. Li, A.J. Merer and C. Thambir 152 (1991) 391
Heavy ions in mixtures of light gases: Fokker–Planck equation and its solution, L. Ferrari 153 (1991) 115
A dipolar chain model for the electrostatics of transmembrane ion channels, M.B. Partenskii, M. Cai and P.C. Jordan 153 (1991) 125
The magnetizability and *g*-factor surfaces of ammonia, S.P.A. Sauer, V. Špirko and J. Oddershede 153 (1991) 189
Xerographic dark discharge of PVK:TNF photoconductive material, J.-Y. Moisan, B. André and R. Lever 153 (1991) 305
Ferromagnetism of charge-transfer crystals, A.L. Tchougreeff and I.A. Misurkin 153 (1991) 371
Electron spin exchange in micellized radical pairs. I. ^{13}C low field chemically induced dynamic nuclear polarization (CIDNP) and ^{13}C radio frequency stimulated nuclear polarization (SNP), I.A. Shkrob, V.F. Tarasov and E.G. Bagryanskaya 153 (1991) 427
Electron spin exchange in micellized radical pairs. II. Magnetic field and magnetic isotope effects in multinuclear pairs, I.A. Shkrob, V.F. Tarasov and A.L. Buchachenko 153 (1991) 443
Xerographic discharge of organic thermoplastic material, J.Y. Moisan, B. André, R. Lever and C. Servens 153 (1991) 465
Model calculations of the anthracene photocurrent spectrum, P. Petelenz and D. Mucha 154 (1991) 145
A dipolar chain model for the electrostatics of transmembrane ion channels, Chem. Phys. 153 (1991) 125–131. Erratum, M.B. Partenskii, M. Cai and P.C. Jordan 154 (1991) 197
A theoretical study on the internal rotation and hyperfine structures of the ethyl radical (CH_3–CH_2), H.U. Suter and T.K. Ha 154 (1991) 227

Motion and geminal recombination of charged carriers in highly anisotropic three-dimensional systems (Onsager theory), G.A. Vinogradov, V.N. Likhachev and A.A. Ovchinnikov 154 (1991) 367
Semiempirical electrostatic polarization model of the ionic bonding in alkali and alkaline earth hydroxides and halides, J.M. Mestdagh and J.P. Visticot 155 (1991) 79
A model description of charge carrier transport phenomena in organic molecular crystals. II. Perylene, E.A. Silinsh, G.A. Shlihta and A.J. Jurgis 155 (1991) 389
Ab initio calculation of phosphorus NMR chemical shifts in the gauge including atomic orbital method, D.B. Chesnut and B.E. Rusiloski 157 (1991) 105
Interaction potentials in rare gas–halide ion systems, V. Kellö and A.J. Sadlej 157 (1991) 123
Ground state electric properties of NaH, G.H.F. Diercksen and A.J. Sadlej 158 (1991) 9
Electric properties of ionic diatoms: BeO, G.H.F. Diercksen, A.J. Sadlej and M. Urban 158 (1991) 19
Charged substituents and the effect of their electric field on the electronic spectra of some aminocoumarins, S.I. Druzhinin, B.D. Bursulaya and B.M. Uzhinov 158 (1991) 137
^{23}Na relaxation in DNA solutions. Influence of intercalation on correlation times and coupling constants, M. Hald and J.P. Jacobsen 159 (1992) 257
The structure and dynamics of 1,3,5-cycloheptatriene and 1,3-cycloheptadiene radical cations in low temperature matrices. An ESR investigation, Y. Kubozono, T. Miyamoto, M. Aoyagi, M. Ata, Y. Matsuda, Y. Gondo, H. Nakamura and T. Matsuo 160 (1992) 421

Spin splittings
EPR investigation of chromium(III) complexes: analysis of their frozen solution and magnetically dilute powder spectra, R.P. Bonomo, A.J. Di Bilio and F. Riggi 151 (1991) 323
Anomalous structure in the $A^6\Sigma^+$–$X^6\Sigma^+$ transition of MnO caused by interference between two internal hyperfine perturbations, A.G. Adam, Y. Azuma, H. Li, A.J. Merer and C. Thambir 152 (1991) 391
Structure of MQ-NMR spin spaces under higher $\mathcal{S}_n$- and $(\mathcal{S}_n)_\downarrow\mathcal{G}$ symmetries. II. $\Gamma/\tilde{\Gamma}$ $(\mathcal{S}_6)_\downarrow\mathcal{O}$ subduced irreps for sixfold spin clusters pertaining to the molecular cage ion, $[^{11}BH]_6^{2-}$, J.P. Colpa and F.P. Temme 154 (1991) 97
Structure of MQ-NMR spin spaces under higher $\mathcal{S}_n$- and $(\mathcal{S}_n)_\downarrow\mathcal{G}$ symmetries. III. $\Gamma/\tilde{\Gamma}$ $((\mathcal{S}_7)_\downarrow D_5)$ subduced irreps for $[A]_7$ clusters pertaining to the molecular cage ion, $[^{11}BH]_7^{2-}$, F.P. Temme and J.P. Colpa 154 (1991) 111
Energy levels of Cr^{3+} ions in C_{3i} sites of $Y_3Al_5O_{12}$, C.A. Morrison, J.B. Gruber and M.E. Hills 154 (1991) 437
Nuclear quadrupole coupling constants of rovibrational levels of all isotopic species of BH^+ in their $X^2\Sigma^+$ and $B'^2\Sigma^+$ states, J. Vojtík, L. Češpiva, I. Paidarová and J. Šavrda 156 (1991) 369
Structure of MQ-NMR spin spaces under higher $\mathcal{S}_n$- and $(\mathcal{S}_n)_\downarrow\mathcal{G}$ symmetries. II. $\Gamma/\tilde{\Gamma}$ $(\mathcal{S}_6)_\downarrow\mathcal{O}$ subduced irreps for sixfold spin clusters pertaining to the molecular cage ion, $[^{11}BH]_6^{2-}$, Chem. Phys. 154 (1991) 97–110. Erratum, J.P. Colpa and F.P. Temme 156 (1991) 532
Theory and simulation of optically induced line shifts in NMR, M.W. Evans 157 (1991) 1
Optically detected magnetic resonance study of the phosphorescent states of trans-2,2′-bipyridine, metal-free cis-2,2′-bipyridine and $[Zn(bpy)]^{2+}$, M. Yagi, B.D. Schlyer and A.H. Maki 157 (1991) 209
Spinning-rate depedence of ^{31}P magic-angle-spinning nuclear magnetic resonance spectra in condensed phosphates, S. Hayashi and K. Hayamizu 157 (1991) 381
The formulae for calculation of *g*-tensor shifts in third-order perturbation theory, E.N. Heifets 160 (1992) 363

Optical activity

Symmetry and magnetic vibrational circular dichroism spectra of a doubly degenerate vibration and its combinations with non-degenerate vibrational modes, M. Pawlikowski and O. Sonnich Mortensen 151 (1991) 73

Circular birefringence and dichroism due to shear stress: optical measurement of non-Newtonian viscosity, M.W. Evans 154 (1991) 193

On the critical scattering phenomena of a nonpolar fluid composed of chiral molecules, E.-K. Lee, D.J. Lee and S.K. Kim 157 (1991) 135

Molecular interactions

A multisurface classical trajectory study of the dynamics of the reaction $O(^1D_2)+H_2\rightarrow OH(v', J', \Theta')+H$ using the diatomics in molecules method, P.J. Kuntz, B.I. Niefer and J.J. Sloan 151 (1991) 77

Model study of the effect of anisotropy on the differential cross section for atom–molecule scattering: the double rainbows, R. Düren, R.K.B. Helbing and S. Milošević 151 (1991) 287

The submillimeter rotation-tunneling spectrum of Ar–D_2O and Ar–NH_3, E. Zwart and W.L. Meerts 151 (1991) 407

Nonexponential solvation dynamics of simple liquids and mixtures, W. Jarzeba, G.C. Walker, A.E. Johnson and P.F. Barbara 152 (1991) 57

An extended diatomics-in-molecules model for NH_2^+, R. Polák 153 (1991) 91

Relaxation cross sections for transfer of rotational angular momentum in a semiclassical approximation, A.V. Storozhev and M.L. Strekalov 153 (1991) 99

The correlated molecular electrostatic potential and electric field of 2(1H)-pyrimidone and 2-hydroxypyrimidine, A. Leś and L. Adamowicz 153 (1991) 409

The $C(^3P_J)+NO(X^2\Pi_r)\rightarrow CN(X^2\Sigma^+)+O(^3P_J)$ reaction dynamics studied at 0.06 and 0.23 eV relative translational energy in pulsed crossed supersonic molecular beams, C. Naulin, M. Costes and G. Dorthe 153 (1991) 519

High pressure study of intermolecular resonance interaction in a naphthalene crystal, K.P. Meletov 154 (1991) 469

An electrostatic-surface stability interpretation of the "hydrophobic" force inferred to occur between mica plates in solutions of soluble surfactants, R. Podgornik and V.A. Parsegian 154 (1991) 477

Chiral discrimination: a model for the interaction between an helicoidal system and an amino acid molecule, E. Alvira, J. Breton, J. Plata and C. Girardet 155 (1991) 7

Semiempirical electrostatic polarization model of the ionic bonding in alkali and alkaline earth hydroxides and halides, J.M. Mestdagh and J.P. Visticot 155 (1991) 79

Experimental determination of the range of interactions of dipole moments in a liquid, J.J. Makosz 155 (1991) 285

New Monte Carlo simulations of many-particle stochastic dynamics: growth of correlations and local self-ordering during annihilation of like particles, R. Brown and N.A. Efremov 155 (1991) 357

Molecular dynamics simulation of crystalline imidazole, S. Besnainou, G. Cardini and D.A. Dows 156 (1991) 71

New mechanism for the vibrational mode-specific proton-transfer reaction $NH_3^+(v)+NH_3\rightarrow NH_2+NH_4^+$, A. Tachibana, T. Suzuki, N. Yoshida, Y. Teramoto and T. Yamabe 156 (1991) 79

Pressure dependence of the polarized reflectance spectrum of a solid charge-transfer complex, perylene-hexacyanobutadiene (HCBD), T. Ida, K. Yakushi, H. Kuroda, H. Yamochi and G. Saito 156 (1991) 113

Isomer-specific radiative lifetimes of molecular heteroclusters, D. Bahatt, U. Even, E. Shalev, N. Ben-Horin and J. Jortner 156 (1991) 223
Electronic spectra and proton transfer in the phenol/$(NH_3)_n$ clusters in argon matrices, C. Crépin and A. Tramer 156 (1991) 281
Vibrational relaxation of glyoxal in collisions with He and Ar, G.-J. Kroes and R.P.H. Rettschnick 156 (1991) 293
State-to-state cross sections for rotational excitation of ortho- and para-NH_3 by He and H_2, J. Schleipen and J.J. ter Meulen 156 (1991) 479
Modified version of the trajectory surface leaking method for dynamical calculations on autoionizing atom–diatom collision systems, J. Vojtík and I. Paidarová 157 (1991) 67
The condensed phases of pyrazine: a test of the Williams–Weller intermolecular potential, Z. Gamba 158 (1991) 59
Proton-transfer dynamics in the hydrogen bond. Inelastic neutron scattering, infrared and Raman spectra of $KH(CF_3COO)_2$ and $CsH(CF_3COO)_2$, F. Fillaux and J. Tomkinson 158 (1991) 113
Protein relaxation dynamics in human myoglobin, D.G. Lambright, S. Balasubramanian and S.G. Boxer 158 (1991) 249
Collision-induced emission of $O_2(a\,^1\Delta_g \rightarrow X\,^3\Sigma_g^-)$ in the gas phase, J. Wildt, E.H. Fink, P. Biggs, R.P. Wayne and A.F. Vilesov 159 (1992) 127
Site effects in spectra of matrix-isolated diatomic molecules: a modelling approach, M. Winter, K. Seranski and U. Schurath 159 (1992) 235
A matrix isolation study of the water–formaldehyde complex. The far-infrared region, B. Nelander 159 (1992) 281
Test of effective pair potential models by molecular dynamics simulation on liquid OCS, J. Samios, H. Stassen and T. Dorfmüller 160 (1992) 33
On the mechanism of radiationless deactivation of rhodamines, T. López Arbeloa, F. López Arbeloa, P.H. Bartolomé and I. López Arbeloa 160 (1992) 123

Spectral bandshapes and intensities

Calculation of the vibrational frequency and line strength versus applied field of carbon monoxide, J.L. Andrés, M. Duran, A. Lledós and J. Bertrán 151 (1991) 37
EPR investigation of chromium(III) complexes: analysis of their frozen solution and magnetically dilute powder spectra, R.P. Bonomo, A.J. Di Bilio and F. Riggi 151 (1991) 323
Excitation and ionization of freon molecules. II. Absolute oscillator strengths for the photoabsorption (7.5–200 eV) and the ionic photofragmentation (12.5–80 eV) of CF_3Cl, W. Zhang, G. Cooper, T. Ibuki and C.E. Brion 151 (1991) 343
Excitation and ionization of freon molecules. III. Absolute oscillator strengths for the photoabsorption (8.5–200 eV) and the ionic photofragmentation (11.5–70 eV) of CF_2Cl_2, W. Zhang, G. Cooper, T. Ibuki and C.E. Brion 151 (1991) 357
Frequency-dependent solvent friction and torsional damping in liquid 1,2-difluoroethane, R.A. MacPhail and F.C. Monroe 152 (1991) 93
On the Jahn–Teller coupling of an orbital triplet with a vibrational doublet, E. Ghelichkhani and E.R. Grant 153 (1991) 133
Doppler-free radio frequency lineshape theory for a three-level system with three allowed transitions in presence of an IR pump, S. Ghoshal and A. Datta 153 (1991) 161
Dissociative excitation of hydrogen in rf and dc glow discharges through H_2, S.B. Vrhovac, S.B. Radovanov, S.A. Bzenić, Z.Lj. Petrović and B.M. Jelenković 153 (1991) 233

Highly excited states of nitric oxide studied by high-resolution resonance-enhanced multiphoton ionization spectroscopy, Y. Luo, Y.D. Cheng, H. Ågren, R. Maripuu, W. Seibt, L. Öhlund, P. Ejeklint, B. Carman, K.Z. Xing, Y. Achiba and K. Siegbahn 153 (1991) 473
Excitation and ionization of freon molecules. IV. Absolute oscillator strengths for the photoabsorption (6–200 eV) and the ionic photofragmentation (11.5–49 eV) of $CFCl_3$, W. Zhang, G. Cooper, T. Ibuki and C.E. Brion 153 (1991) 491
Effects of homogeneous and inhomogeneous broadening mechanisms and molecular rearrangement dynamics on frequency resolved and time resolved coherent Raman intensities, H. Okamoto 155 (1991) 291
A vibrational study of the CD_3H molecule in the curvilinear formulation, C. Iung and C. Leforestier 155 (1991) 369
Vibronic coupling in Rydberg series of linear molecules, A. Staib, W. Domcke and A.L. Sobolewski 156 (1991) 21
Theoretical study of multiple-scattering effects in the X-ray absorption spectra of iron-porphyrins, F. Bohr and M.F. Ruiz-López 156 (1991) 55
Dissociation of aliphatic hydrocarbons excited by electrons: translational energy distributions of the excited hydrogen atom, T. Ogawa, T. Tsuboi and K. Nakashima 156 (1991) 465
Dissociation of hydrogen sulfide in e–H_2S collisions: translational energy distribution of $H^*(n=4)$, T. Ogawa, M. Tsukada and K. Nakashima 156 (1991) 473
Optothermal-detected microwave-sideband CO_2-laser spectroscopy of NCH–NH_3, G.T. Fraser, A.S. Pine, W.A. Kreiner and R.D. Suenram 156 (1991) 523
Transition probabilities for the $B\,^1\Delta_g$–$A\,^1\Pi_u$ and $B'\,^1\Sigma_g^+$–$A\,^1\Pi_u$ infrared bands of C_2. An ab initio study, P.J. Bruna and J.S. Wright 157 (1991) 111
Absorption spectra of a solvated electron in ethers, H. Abramczyk and J. Kroh 157 (1991) 373
Driven damped harmonic oscillators perturbed by the parity operator, P. Blaise, M. Giry and O. Henri-Rousseau 159 (1992) 169
Characterization of the $\tilde{B}\leftarrow\tilde{X}$ transition of the chlorobenzene cation prepared in non-equilibrium rotational population distributions by resonance enhanced multiphoton ionization, F. Morlet-Savary, I. Dimicoli, C. Cossart-Magos and J.E. Parkin 159 (1992) 303
Computational experiments on the intramolecular energy flow in macromolecules, B.G. Sumpter and D.W. Noid 160 (1992) 393
The structure and dynamics of 1,3,5-cycloheptatriene and 1,3-cycloheptadiene radical cations in low temperature matrices. An ESR investigation, Y. Kubozono, T. Miyamoto, M. Aoyagi, M. Ata, Y. Matsuda, Y. Gondo, H. Nakamura and T. Matsuo 160 (1992) 421
Absolute dipole differential oscillator strengths for inner shell spectra from high resolution electron energy loss studies of the freon molecules CF_4, CF_3Cl, CF_2Cl_2, $CFCl_3$ and CCl_4, W. Zhang, T. Ibuki and C.E. Brion 160 (1992) 435
Electronic spectra and transitions of the fullerene C_{60}, S. Leach, M. Vervloet, A. Desprès, E. Bréheret, J.P. Hare, T.J. Dennis, H.W. Kroto, R. Taylor and D.R.M. Walton 160 (1992) 451

Coupling of electronic and nuclear motion

Model studies on femtosecond time-resolved ionization spectroscopy of excited-state vibrational dynamics and vibronic coupling, M. Seel and W. Domcke 151 (1991) 59
Picosecond Stokes shift studies of solvent friction: experimental measurements of time-dependent band shape and integrated intensity, J.D. Simon and S.-G. Su 152 (1991) 143
On the Jahn–Teller coupling of an orbital triplet with a vibrational doublet, E. Ghelichkhani and E.R. Grant 153 (1991) 133

Anomalous magnetic effects. The role of association in the recombination of singlet radical pairs in liquids, N.V. Shokhirev, E.C. Korolenko, M.B. Taraban and T.V. Leshina 154 (1991) 237
The optical spectrum of $Ba_2Zn[Cu]F_6$, D. Reinen, G. Steffen, M.A. Hitchman, H. Stratemeier, L. Dubicki, E.R. Krausz, M.J. Riley, H.E. Mathies, K. Recker and F. Wallrafen 155 (1991) 117
Symmetry and vibronic coupling: the stereochemistry and the ground state potential surface of Cu^{2+} in five-coordination, D. Reinen and M. Atanasov 155 (1991) 157
Theoretical study of the $HeH(B^2\Pi)$ fluorescence and predissociation, A.B. Alekseyev, V.S. Ivanov, A.M. Pravilov and O.D. Shestakov 155 (1991) 173
Electron transfer induced by liquid defect motion. Exact solution, D.V. Matyushov 155 (1991) 331
Vibronic coupling in Rydberg series of linear molecules, A. Staib, W. Domcke and A.L. Sobolewski 156 (1991) 21
Dissipative relaxation of a low-energy intermediate electronic state in three-level electron transfer, A.M. Kuznetsov and J. Ulstrup 157 (1991) 25
Absorption spectra of a solvated electron in ethers, H. Abramczyk and J. Kroh 157 (1991) 373
The dynamics of the primary event in rhodopsins revisited, A. Warshel, Z.T. Chu and J.-K. Hwang 158 (1991) 303
MO LCAO analysis of the vibronic instability of the $CuCl_5^{3-}$ trigonal bipyramidal configuration. Critical view on the angular overlap model in vibronic problems, V.Z. Polinger, N.N. Gorinchoi and I.B. Bersuker 159 (1992) 75
Fluorescence excitation spectrum of 1,8-disubstituted naphthalenes in supersonic jet, T. Chakraborty and M. Chowdhury 159 (1992) 439
Ab initio study of the vibrational structure of the X^2A_1 and A^2B_1 electronic states of CH_2^+, W. Reuter and S.D. Peyerimhoff 160 (1992) 11

Energy transfer processes

Time-dependent fluorescence depolarization arising from exciton annihilation in confined molecular domains, G. Juzeliūnas 151 (1991) 169
Quenching and rotational transfer rates in the $v'=0$ manifold of $OH(A^2\Sigma^+)$, J. Burris, J. Butler, T. McGee and W. Heaps 151 (1991) 233
Degenerate triplet spin exchange in liquid solution studied by pulse NMR, J. Burri and H. Fischer 151 (1991) 279
A study of the S_1 $6^1(^1A_2'')$ vibronically excited state of sym-triazine by high-resolution UV laser spectroscopy, P. Uijt de Haag, W.L. Meerts and J.T. Hougen 151 (1991) 371
Secondary heating effects in laser-induced fluorescence experiments, K.L. McNesby and R.D. Bates Jr. 151 (1991) 385
CO_2 laser-induced fluorescence studies of vibrational energy transfer in N_2O, K.L. McNesby and R.D. Bates Jr. 151 (1991) 401
Near- and non-resonant (VV) energy transfer between molecules dissolved in liquid krypton: a comparison with liquid argon, J.J. Andrew, D.C. McDermott, S.P. Mills and C.J.S.M. Simpson 153 (1991) 247
Core excitation-induced photodesorption of molecular and fragment ions from CO adsorbates on metal surfaces, R. Treichler, W. Wurth, W. Riedl, P. Feulner and D. Menzel 153 (1991) 259
A femtosecond study of electronic state dynamics of fucoxanthin and implications for photosynthetic carotenoid-to-chlorophyll energy transfer mechanisms, A.P. Shreve, J.K. Trautman, T.G. Owens and A.C. Albrecht 154 (1991) 171

Vibrational energy transfer in the N_2^*–OCS system. Measurements of vibrational populations of the bending manifold in the perturbed steady state by microwave spectroscopy, L.B. Favero, M.C. Righetti and P.G. Favero 155 (1991) 107
Spatial distribution of probes in a micelle: effects on the energy transfer time-resolved measurables, A.V. Barzykin 155 (1991) 221
Fluorescence depolarization in nonlinear molecular pairs, D. Gülen 156 (1991) 123
Vibrational relaxation of glyoxal in collisions with He and Ar, G.-J. Kroes and R.P.H. Rettschnick 156 (1991) 293
Theory of diffusion-influenced fluorescence quenching: dependence of the Stern–Volmer curve on light intensity, S. Lee, M. Yang, K.J. Shin, K.Y. Choo and D. Lee 156 (1991) 339
State-to-state cross sections for rotational excitation of ortho- and para-NH_3 by He and H_2, J. Schleipen and J.J. ter Meulen 156 (1991) 479
Laser excitation of the $A^3\Sigma_u^+$, $A'^3\Delta_u$ and $c^1\Sigma_u^-$ states of molecular oxygen, J. Wildt, G. Bednarek, E.H. Fink and R.P. Wayne 156 (1991) 497
Dissociation rate and N(^{4}S) atom concentrations in a N_2 glow-discharge, J. Loureiro 157 (1991) 157
Singlet excitation energy transfer in tetracene doped *p*-terphenyl single crystals, A. Krüger, C. Kryschi, L. Valkunas and D. Schmid 157 (1991) 243
A time-resolved fluorescence study of electronic excitation energy transport in concentrated dye solutions, A.D. Scully, A. Matsumoto and S. Hirayama 157 (1991) 253
Relaxation of singlet molecular oxygen in the liquid and gas phase up to 154 K, M. Seidl, J. Kaa and M. Maier 157 (1991) 279
The He–N_2 interaction revisited: a comparison of measured and computed differential cross sections, F.A. Gianturco, A. Palma and N. Sanna 158 (1991) 77
Angular momentum and rotational energy relaxation in N_2–N_2 collisions calculated from coherent and stimulated Raman spectroscopy data, S. Temkin, J.M. Thuet, L. Bonamy, J. Bonamy and D. Robert 158 (1991) 89
Intramultiplet relaxation of Cd(5^3P_2) induced by collisions with N_2 and CO, A. Masaki, T. Ohnuma, K. Kuwahara, H. Umemoto, Y. Wada, F. Misaizu and K. Fuke 158 (1991) 155
Molecular dynamics study of the photodissocation of carbon monoxide from myoglobin: ligand dynamics in the first 10 ps, J.E. Straub and M. Karplus 158 (1991) 221
Optical and ODMR spectroscopy of an induced triplet X-trap in 1,4-dibromobenzene single crystals, B. Stein, F. Rothamel, T. Kirski, J. Kolenda and C. von Borczyskowski 159 (1992) 269
Energy transfer distributions for classical, collinear atom–diatom collisions, N. Snider 159 (1992) 339
Sub-picosecond time-resolved IR spectroscopy of the vibrational dynamics of $Rh(CO)_2(acac)$, J.D. Beckerle, M. Casassa, R.R. Cavanagh, E.J. Heilweil and J.C. Stephenson 160 (1992) 487

Molecular photophysical processes

Trans–cis photoisomerization mechanism of carbocyanines: experimental check of theoretical models, G. Ponterini and F. Momicchioli 151 (1991) 111
Spectroscopy and relaxation dynamics of metastable electronically excited states of iodine in rare gas matrices, M. Macler and M.C. Heaven 151 (1991) 219
Triplet electron–proton cross-polarization by satisfying a modified Hartmann–Hahn condition, R.H. Fritsch, H. Brunner and K.H. Hausser 151 (1991) 261
Excitation and ionization of freon molecules. II. Absolute oscillator strengths for the photoabsorption (7.5–200 eV) and the ionic photofragmentation (12.5–80 eV) of CF_3Cl, W. Zhang, G. Cooper, T. Ibuki and C.E. Brion 151 (1991) 343

Excitation and ionization of freon molecules. III. Absolute oscillator strengths for the photoabsorption (8.5–200 eV) and the ionic photofragmentation (11.5–70 eV) of CF_2Cl_2, W. Zhang, G. Cooper, T. Ibuki and C.E. Brion 151 (1991) 357
Rovibronic level structure of electronically excited acetylene ($\tilde{A}\,^1A_u$) in a supersonic jet as studied by laser-induced fluorescence and Zeeman quantum beat spectroscopy, N. Ochi and S. Tsuchiya 152 (1991) 319
Transient spectroscopy of triphenylmethane derivatives following subpicosecond irradiation, M.M. Martin, P. Plaza and Y.H. Meyer 153 (1991) 297
Excitation and ionization of freon molecules. IV. Absolute oscillator strengths for the photoabsorption (6–200 eV) and the ionic photofragmentation (11.5–49 eV) of $CFCl_3$, W. Zhang, G. Cooper, T. Ibuki and C.E. Brion 153 (1991) 491
Theoretical study of the electronic spectrum of ammonia: generalized oscillator strength calculations for the A–X transition, L. Chantranupong, G. Hirsch, R.J. Buenker, M. Kimura and M.A. Dillon 154 (1991) 13
Photochromic thiophenefulgides. Photokinetics of two isopropyl derivatives, K. Ulrich, H. Port, H.C. Wolf, J. Wonner, F. Effenberger and H.-D. Ilge 154 (1991) 311
Oxygen K-shell excitation spectroscopy of hydrogen peroxide, E. Rühl and A.P. Hitchcock 154 (1991) 323
On the validity of the RWA for steady state and temporal populations of molecular states involved in IR multi-photon excitations, S. Nakai and W.J. Meath 154 (1991) 349
Excimer geometries in bichromophoric molecules: a theoretical and experimental study of 1,2-(bis-9-antrhyl)-ethane, G.D. Scholes, K.P. Ghiggino and G.J. Wilson 155 (1991) 127
Experimental and theoretical study of the N_{1s} and C_{1s} shake-up satellites in pyridine and aniline, M.P. Keane, A. Naves de Brito, N. Correia, S. Svensson and S. Lunell 155 (1991) 379
Laser-initiated chain reactions and microexplosions in solid solutions of methylcyclopropane and chlorine, T.J. Tague Jr. and C.A. Wight 156 (1991) 141
Energy and rotational state dependence of radiationless processes in propynal, P.R. Willmott, H. Bitto and J.R. Huber 156 (1991) 177
Vibrational and rotational effects on the intersystem crossing in pyrazine and pyrimidine, P. Uijt de Haag and W.L. Meerts 156 (1991) 197
Isomer-specific radiative lifetimes of molecular heteroclusters, D. Bahatt, U. Even, E. Shalev, N. Ben-Horin and J. Jortner 156 (1991) 223
Fluorescence analysis of two new TICT systems: 10-cyano-9,9′-bianthryl (CBA) and 10,10′-dicyano-9,9′-bianthryl (DCBA), S. Müller and J. Heinze 157 (1991) 231
The effect of pressure on the dynamic quenching by oxygen of the excited singlet state of 9,10-dimethylanthracene in solution, A.D. Scully, H. Yasuda, M. Okamoto and S. Hirayama 157 (1991) 271
Laser-initiated chain reactions and microexplosions in solid solutions of methylcyclopropane and chlorine, Chem. Phys. 156 (1991) 141–148. Erratum, T.J. Tague Jr. and C.A. Wright 157 (1991) 305
General numerical solution to the time-dependent master equation for non-steady-state reactions: application to the photoinitiated isomerization of cycloheptatriene to toluene, R.L. Jackson 157 (1991) 315
Variational approach to quantum dynamics: a simple application to molecular photodissociation, G.P. Arrighini, N. Durante and C. Guidotti 157 (1991) 365
On the fluorescence depolarization in bis-(N-carbazolyl) compounds, M. Hennecke and H.F. Kauffmann 157 (1991) 391
Photothermal grating spectroscopy study of nongeminate atom recombination of photodissociated iodine in liquids, X.R. Zhu and J.M. Harris 157 (1991) 409

Evidence for proximal control of ligand specificity in hemeproteins: absorption and Raman studies of cryogenically trapped photoproducts of ligand bound myoglobins, A.M. Ahmed, B.F. Campbell, D. Caruso, M.R. Chance, M.D. Chavez, S.H. Courtney, J.M. Friedman, I.E.T. Iben, M.R. Ondrias and M. Yang 158 (1991) 329
Theoretical and experimental study on the electronic spectrum and photophysics of Michler's hydrol blue, I. Baraldi, A. Carnevali, F. Momicchioli and G. Ponterini 160 (1992) 85
On the photo-sensitized injection of electrons into SnO_2 from cyanine dyes incorporated in Langmuir–Blodgett films, G. Biesmans, M. Van der Auweraer, C. Cathry, F.C. De Schryver, Y. Yonezawa and T. Sato 160 (1992) 97
On the mechanism of radiationless deactivation of rhodamines, T. López Arbeloa, F. López Arbeloa, P.H. Bartolomé and I. López Arbeloa 160 (1992) 123
Principal-component self-modeling analysis of fluorescence for some trans-diarylethylenes. A comparison with kinetic analysis, A. Spalletti, G. Bartocci, F. Masetti, U. Mazzucato and G. Cruciani 160 (1992) 131
Temperature dependence of the fluorescence spectra of poly-N-vinylcarbazole films from 300 to 550 K: evidence for monomer emission, G. Giro and G. Orlandi 160 (1992) 145
Generalized golden rule approach to the H-transfer problem. II. Application to a photochemical reaction, L. Lavtchieva and Z. Smedarchina 160 (1992) 211
Intramolecular charge transfer and trans–cis isomerization of the DCM styrene dye in polar solvents. A CS INDO MRCI study, S. Marguet, J.C. Mialocq, P. Millie, G. Berthier and F. Momicchioli 160 (1992) 265
Absolute dipole differential oscillator strengths for inner shell spectra from high resolution electron energy loss studies of the freon molecules CF_4, CF_3Cl, CF_2Cl_2, $CFCl_3$ and CCl_4, W. Zhang, T. Ibuki and C.E. Brion 160 (1992) 435

Intramolecular dynamics

A multisurface classical trajectory study of the dynamics of the reaction $O(^1D_2)+H_2\rightarrow OH(v', J', \Theta')+H$ using the diatomics in molecules method, P.J. Kuntz, B.I. Niefer and J.J. Sloan 151 (1991) 77
Anomalous behavior of the anticrossing density as a function of excitation energy in the C_2H_2 molecule, P. Dupré, R. Jost, M. Lombardi, P.G. Green, E. Abramson and R.W. Field 152 (1991) 293
Quantum effects in competitive unimolecular reactions, F. Remacle, M. Desouter-Lecomte and J.C. Lorquet 153 (1991) 201
Anomalous behaviour of the anticrossing density as a function of excitation energy in the C_2H_2 molecule, Chem. Phys. 152 (1991) 293. Erratum, P. Dupré, R. Jost, M. Lombardi, P.G. Green, E. Abramson and R.W. Field 153 (1991) 539
A femtosecond study of electronic state dynamics of fucoxanthin and implications for photosynthetic carotenoid-to-chlorophyll energy transfer mechanisms, A.P. Shreve, J.K. Trautman, T.G. Owens and A.C. Albrecht 154 (1991) 171
Isomerization and unimolecular rearrangement channels of dithioformic acid, Y. Tao 154 (1991) 221
Quantum kinetic energy operator for a group of particles in terms of scalar basic rotational invariant coordinates derived from a generalized Jacobi vector (GJV) description. III. A metric tensors approach, J.P. Leroy, H. Rabitz and R. Wallace 154 (1991) 395
Excimer geometries in bichromophoric molecules: a theoretical and experimental study of 1,2-(bis-9-antrhyl)-ethane, G.D. Scholes, K.P. Ghiggino and G.J. Wilson 155 (1991) 127
Translational energy study of CH_3 photofragments following $^1(n,\pi^*)$ excitation of acetone, L.D. Waits, R.J. Horwitz and J.A. Guest 155 (1991) 149

The phase space moment method for studying intramolecular vibrational energy redistribution, G. Huacai and J. Fenglin 155 (1991) 345
Real-time dynamics of vibrational predissociation in anthracene–Ar_n (n=1,2,3), A. Heikal, L. Bañares, D.H. Semmes and A.H. Zewail 156 (1991) 231
Many-body calculations of the core hole spectra of NiCO, M. Ohno and P. Decleva 156 (1991) 309
Optically detected magnetic resonance study of the phosphorescent states of trans-2,2′-bipyridine, metal-free cis-2,2′-bipyridine and $[Zn(bpy)]^{2+}$, M. Yagi, B.D. Schlyer and A.H. Maki 157 (1991) 209
The vibrational constant of the $O_2^{2+}X\,^1\Sigma_g^+$ state from the dissociative decay of n=3,4 Rydberg states in O_2^+, W.J. van der Zande 157 (1991) 287
Hydrogen-exchange labeling study of the allosteric R-state to T-state equilibrium in methemoglobin, R.E. McKinnie, J.J. Englander and S.W. Englander 158 (1991) 283
Time- and temperature dependence of large-scale conformational transitions in myoglobin, R.D. Young, H. Frauenfelder, J.B. Johnson, D.C. Lamb, G.U. Nienhaus, R. Philipp and R. Scholl 158 (1991) 315
A molecular dynamics simulation of the C-terminal fragment of the L7/L12 ribosomal protein in solution, V. Daggett and M. Levitt 158 (1991) 501
From cluster to crystal: ab initio calculations of the OH^- frequency in lithium hydroxide monohydrate, K. Hermansson 159 (1992) 67
A semiclassical simulation for tunneling dynamics of malonaldehyde and hydrogenoxalate anion, E. Bosch, M. Moreno and J.M. Lluch 159 (1992) 99
The dynamics of dressed variables, D.M. Charutz and R.D. Levine 159 (1992) 321
A weak-mode representation of floppy molecules. I. Potential energy, C. Saint-Espès, X. Chapuisat and F. Schneider 159 (1992) 377
A weak-mode representation of floppy molecules. II. Kinetic energy and total Hamiltonian matrix, X. Chapuisat and C. Saint-Espès 159 (1992) 391
The Pariser–Parr–Pople model for trans-polyenes. II. Parametrization and ground state dynamics, W. Förner 160 (1992) 189

–radiationless transitions
Optical potentials by the complex coordinate method, N. Rom, N. Lipkin and N. Moiseyev 151 (1991) 199
A study of the S_1 $6^1(^1A_2'')$ vibronically excited state of sym-triazine by high-resolution UV laser spectroscopy, P. Uijt de Haag, W.L. Meerts and J.T. Hougen 151 (1991) 371
S_1–T_1 coupling in propynal by level anticrossing spectroscopy, M. Lombardi, J.P. Pique, U. Brühlmann and J.R. Huber 156 (1991) 163
Energy and rotational state dependence of radiationless processes in propynal, P.R. Willmott, H. Bitto and J.R. Huber 156 (1991) 177
On the mechanism of radiationless deactivation of rhodamines, T. López Arbeloa, F. López Arbeloa, P.H. Bartolomé and I. López Arbeloa 160 (1992) 123

–vibrational energy redistribution (including vibrational dissociation)
Mixing of the vibrational angular momentum components of multiply degenerate vibronic states of benzene by vibrational *l*-type resonance, E. Riedle and J. Pliva 152 (1991) 375
Quantum effects in competitive unimolecular reactions, F. Remacle, M. Desouter-Lecomte and J.C. Lorquet 153 (1991) 201
Connecting level statistics and reaction dynamics: mode selective decay of resonant states for HXXH-type molecules, B. Hartke and W. Karrlein 154 (1991) 63

Vibrational energy transfer in the N_2^*–OCS system. Measurements of vibrational populations of the bending manifold in the perturbed steady state by microwave spectroscopy, L.B. Favero, M.C. Righetti and P.G. Favero 155 (1991) 107
The phase space moment method for studying intramolecular vibrational energy redistribution, G. Huacai and J. Fenglin 155 (1991) 345
A vibrational study of the CD_3H molecule in the curvilinear formulation, C. Iung and C. Leforestier 155 (1991) 369
Dissociation rate and $N(^4S)$ atom concentrations in a N_2 glow-discharge, J. Loureiro 157 (1991) 157
Molecular dynamics study of the photodissocation of carbon monoxide from myoglobin: ligand dynamics in the first 10 ps, J.E. Straub and M. Karplus 158 (1991) 221
Driven damped harmonic oscillators perturbed by the parity operator, P. Blaise, M. Giry and O. Henri-Rousseau 159 (1992) 169
The importance of periodic orbits in analysing photodissociation resonances: the O_3 case, S.C. Farantos 159 (1992) 329
The dissociation dynamics of low lying triplet states in butane and butene molecules, J.H.M. Beijersbergen, C.G. de Koster, W.J. van der Zande, P.G. Kistemaker and J. Los 160 (1992) 151

Luminescence spectra, yields and lifetimes
Determination of the radiative lifetimes of nine ion-pair states of I_2, P.J. Jewsbury, K.P. Lawley, T. Ridley, F.F. Al-Adel, P.R.R. Langridge-Smith and R.J. Donovan 151 (1991) 103
Time-dependent fluorescence depolarization arising from exciton annihilation in confined molecular domains, G. Juzeliūnas 151 (1991) 169
Spectroscopy and relaxation dynamics of metastable electronically excited states of iodine in rare gas matrices, M. Macler and M.C. Heaven 151 (1991) 219
Chemical reaction rates and solvation dynamics in electrolyte solutions: ion atmosphere friction, G. van der Zwan and J.T. Hynes 152 (1991) 169
Theory of multiquantum optically detected ESR spectra of radical pairs. I. General theory. Resonances in parallel radio-frequency field, V.A. Morozov and A.B. Doktorov 153 (1991) 313
Theory of multiquantum optically detected ESR spectra of radical pairs. II. Resonances in perpendicular radio-frequency field, V.A. Morozov and A.B. Doktorov 153 (1991) 333
Theoretical study of the $HeH(B^2\Pi)$ fluorescence and predissociation, A.B. Alekseyev, V.S. Ivanov, A.M. Pravilov and O.D. Shestakov 155 (1991) 173
Magnetic field dependence of rotationally resolved excitation spectra of the $^1B_{3u}$ 0_0^0 transition of jet-cooled pyrazine, P.J. de Lange, H.Th. Jonkman and K.E. Drabe 156 (1991) 209
Theory of diffusion-influenced fluorescence quenching: dependence of the Stern–Volmer curve on light intensity, S. Lee, M. Yang, K.J. Shin, K.Y. Choo and D. Lee 156 (1991) 339
Radiative lifetimes of confined excitations in sigma-conjugated silane oligomers, J.R.G. Thorne, S.A. Williams, R.M. Hochstrasser and P.J. Fagan 157 (1991) 401
Solvatochromatic shifts studied by multi-configuration self-consistent reaction field theory. Application to azabenzenes, H. Ågren, S. Knuts, K.V. Mikkelsen and H.J.Aa. Jensen 159 (1992) 211
CuBr chemiluminescence from the $Cu^*(^2D_{3/2,5/2}) + Br_2$ reaction, P. Kowalczyk, I. Hikmet and N. Sadeghi 160 (1992) 73
Principal-component self-modeling analysis of fluorescence for some trans-diarylethylenes. A comparison with kinetic analysis, A. Spalletti, G. Bartocci, F. Masetti, U. Mazzucato and G. Cruciani 160 (1992) 131
Temperature dependence of the fluorescence spectra of poly-N-vinylcarbazole films from 300 to 550 K: evidence for monomer emission, G. Giro and G. Orlandi 160 (1992) 145

Coherence loss processes
Time-resolved relaxation of one- and two-vibron states in the rubidium perchlorate crystal, G.M. Gale and P. Schanne 151 (1991) 127
Fluorescence detected level-anticrossing and spin coherence of a localized triplet state in diamond, E. van Oort and M. Glasbeek 152 (1991) 365
Optical and ODMR spectroscopy of an induced triplet X-trap in 1,4-dibromobenzene single crystals, B. Stein, F. Rothamel, T. Kirski, J. Kolenda and C. von Borczyskowski 159 (1992) 269

Non-linear responses (including optical)
Conformational dependence of the quadratic hyperpolarisabilities of a series of push–pull diaryl acetylenes: an experimental and computational investigation, M. Barzoukas, A. Fort, G. Klein, A. Boeglin, C. Serbutoviez, L. Oswald and J.F. Nicoud 153 (1991) 457
Resonant degenerate four wave mixing and scaling laws for saturable absorption in thin films of conjugated polymers and Rhodamine 6G, C. Bubeck, A. Kaltbeitzel, A. Grund and M. LeClerc 154 (1991) 343
Simulation of the unstable dynamics of excitable biomembranes: properties of a cyclic electrochemical gating mechanism, K.D. Schulze 156 (1991) 43
Electronic spectra of 4-nitro-pyridine-*n*-oxide (NPO) single crystals, M. Pierre, P.L. Baldeck, D. Block, R. Georges, H.P. Trommsdorff and J. Zyss 156 (1991) 103
Measurement of quadratic hyperpolarizabilities of unsymmetrical donor–acceptor bi- and polyaryls: effect of size and torsion angle of aryl units, G. Puccetti, I. Ledoux, J. Zyss, A. Jutand and C. Amatore 160 (1992) 467
Ab initio calculations on the one- and two-photon electronic transitions of cyclopentadiene, spirononateraene, 1,4-cyclo-hexadiene, Dewar benzene, norbornadiene, and barrelene, V. Galasso 153 (1991) 13
Theory of multiquantum optically detected ESR spectra of radical pairs. I. General theory. Resonances in parallel radio-frequency field, V.A. Morozov and A.B. Doktorov 153 (1991) 313
Theory of multiquantum optically detected ESR spectra of radical pairs. II. Resonances in perpendicular radio-frequency field, V.A. Morozov and A.B. Doktorov 153 (1991) 333
Highly excited states of nitric oxide studied by high-resolution resonance-enhanced multiphoton ionization spectroscopy, Y. Luo, Y.D. Cheng, H. Ågren, R. Maripuu, W. Seibt, L. Öhlund, P. Ejeklint, B. Carman, K.Z. Xing, Y. Achiba and K. Siegbahn 153 (1991) 473
Multiphoton dissociation dynamics of highly excited states of CS_2 and CS_2 clusters, E. Patsilinakou, D. Proch and C. Fotakis 153 (1991) 503
Resonant two-photon ionization of phenol in methylene chloride doped solid argon using 248 nm KrF laser and 254 nm Hg lamp radiation, a comparative study. The UV/VIS absorption spectrum of phenol radical cation, K. Kesper, F. Diehl, J.G.G. Simon, H. Specht and A. Schweig 153 (1991) 511
On the validity of the RWA for steady state and temporal populations of molecular states involved in IR multi-photon excitations, S. Nakai and W.J. Meath 154 (1991) 349
Zeeman effect in the two-photon excitation spectrum of the $C^2\Pi$ state of NO, S. Guizard, N. Shafizadeh, D. Chapoulard, M. Horani and D. Gauyacq 156 (1991) 509

Reactions (including dissociation)
Photoionization mass spectrometry of kinetic energy-selected ions. An ion retarding potential difference method applied to NO^+ and O^+ from N_2O, R. Locht, G. Hagenow, K. Hottmann and H. Baumgärtel 151 (1991) 137
Solvent effect on activated rate processes: on the validity of the GLE approach, G. Tarjus and D. Kivelson 152 (1991) 153

Quasiclassical trajectory study of the two channels of the F+ICl system: effect of the collisional energy, I. Urrecha, I. Serna and J. Iturbe 154 (1991) 85
Dissociative excitation of SiH_4 by electron impact: emission cross sections for the hydrogen Lyman series, S. Tsurubuchi, K. Motohashi, S. Matsuoka and T. Arikawa 155 (1991) 401
Activated rate processes in the multidimensional case. Consideration of recrossings in the multidimensional Kramers problem with anisotropic friction, A.M. Berezhkovskii and V.Yu. Zitserman 157 (1991) 141
Time-dependent calculation of the energy resolved state-to-state transition probabilities for three-atom exchange reactions, M. Monnerville, P. Halvick and J.C. Rayez 159 (1992) 227
Master equation for site distributions describing barrier crossing in the presence of anisotropic diffusion, G.J. Moro 159 (1992) 421
The dissociation dynamics of low lying triplet states in butane and butene molecules, J.H.M. Beijersbergen, C.G. de Koster, W.J. van der Zande, P.G. Kistemaker and J. Los 160 (1992) 151

–gas phase
Hydroxonium ion formation in collisions of $H_2O^+ + D_2O$ and $D_2O^+ + H_2O$: a crossed-beam scattering study, J. Vančura and Z. Herman 151 (1991) 249
Generalized Langevin model for molecular dynamics of an activated reaction in solution, I. Benjamin, L.L. Lee, Y.S. Li, A. Liu and K.R. Wilson 152 (1991) 1
Trajectory capture rate coefficients for ion–quadrupolar molecule reactions, I. Mendaš and P. Milutinović 153 (1991) 73
Production of the N_2 $(A^3\Sigma_u^+)$ metastable state by electron impact dissociative excitation of N_2O, S.M. Barnett, N.J. Mason and W.R. Newell 153 (1991) 283
Theoretical study of the reaction of OH with HNO, M.R. Soto, M. Page and M.L. McKee 153 (1991) 415
Emission of Xe:N(^{2}P) collision complexes near the N(^{2}P→^{2}D) lines, A.F. Vilesov, J. Wildt and E.H. Fink 153 (1991) 531
An experimental and theoretical study of SF^{q+} $(q=1–3)$ ions, K. Nagesha, V.R. Marathe and D. Mathur 154 (1991) 125
Calculation of the inner shell excitation spectra and estimation of the electron scattering and dissociative attachment resonance energies of SF_6, SO_2, SF_2O, SF_2O_2, SF_4, SF_4O and S_2F_{10}, J.A. Tossell 154 (1991) 211
Analytical potential energy surface for methane in terms of interatomic forces, H. Furue, J.F. LeBlanc, P.D. Pacey and J.M. Whalen 154 (1991) 425
Translational energy study of CH_3 photofragments following $^1(n,\pi^*)$ excitation of acetone, L.D. Waits, R.J. Horwitz and J.A. Guest 155 (1991) 149
Dissociative excitation of SiH_4 by electron impact: emission cross sections for the hydrogen Lyman series, S. Tsurubuchi, K. Motohashi, S. Matsuoka and T. Arikawa 155 (1991) 401
New mechanism for the vibrational mode-specific proton-transfer reaction $NH_3^+(v) + NH_3 \rightarrow NH_2 + NH_4^+$, A. Tachibana, T. Suzuki, N. Yoshida, Y. Teramoto and T. Yamabe 156 (1991) 79
Dissociation of aliphatic hydrocarbons excited by electrons: translational energy distributions of the excited hydrogen atom, T. Ogawa, T. Tsuboi and K. Nakashima 156 (1991) 465
Dissociation of hydrogen sulfide in e–H_2S collisions: translational energy distribution of $H^*(n=4)$, T. Ogawa, M. Tsukada and K. Nakashima 156 (1991) 473
Dissociation rate and N(^{4}S) atom concentrations in a N_2 glow-discharge, J. Loureiro 157 (1991) 157
The benzene dication: energies of excited states determined by double-charge-transfer spectroscopy using OH^+ and F^+ projectile ions, W.J. Griffiths and F.M. Harris 157 (1991) 299

General numerical solution to the time-dependent master equation for non-steady-state reactions: application to the photoinitiated isomerization of cycloheptatriene to toluene, R.L. Jackson 157 (1991) 315
Core level photoionization mass spectroscopy of the fluoromethylsilanes, $Si(CH_3)_xF_{4-x}$ ($x=0$–4), around the Si 2p ionization edges, J.D. Bozek, K.H. Tan, G.M. Bancroft and K.J. Fu 158 (1991) 171
Interaction between two chemical reactions in gases. The nonequilibrium effects from the Boltzmann and Fokker–Planck equations within a Lorentz gas model, A.S. Cukrowski, A.L. Kawczyński, J. Popielawski, W. Stiller and R. Schmidt 159 (1992) 39
Quantum-classical reaction path model for chemical reactions. IV. The reaction $Cl^- + CH_3Cl \rightarrow ClCH_3 + Cl^-$, G.D. Billing 159 (1992) 109
Ab-initio multiple reference double-excitation configuration-interaction ground and excited state potential curves for the H_2N–NO_2 decomposition in nitramine, S. Roszak and J.J. Kaufman 160 (1992) 1
Temperature dependence of cyanogen radical reactions with selected alkanes: CN reactivities towards primary, secondary and tertiary C–H bonds, D.L. Yang, T. Yu, N.S. Wang and M.C. Lin 160 (1992) 307
CN radical reactions with selected olefins in the temperature range 174–740 K, D.L. Yang, T. Yu, N.S. Wang and M.C. Lin 160 (1992) 317
Experimental and theoretical investigation of the reaction $CF_3 + NO + M \rightarrow CF_3NO + M$ from 0.5 to 12 Torr and from 253 to 373 K, J. Masanet, F. Caralp, L. Ley and R. Lesclaux 160 (1992) 383

–condensed phase
Generalized Langevin model for molecular dynamics of an activated reaction in solution, I. Benjamin, L.L. Lee, Y.S. Li, A. Liu and K.R. Wilson 152 (1991) 1
An exact theory of friction for reactive collisions in a solvent using an interaction representation, D.M. Charutz and R.D. Levine 152 (1991) 31
Metal carbonyl photochemistry in organic solvents: femtosecond transient absorption and preliminary resonance Raman spectroscopy, A.G. Joly and K.A. Nelson 152 (1991) 69
Solvent cage effects and chemical dynamics in liquids, F. Patron and S.A. Adelman 152 (1991) 121
Solvent effect on activated rate processes: on the validity of the GLE approach, G. Tarjus and D. Kivelson 152 (1991) 153
Chemical reaction rates and solvation dynamics in electrolyte solutions: ion atmosphere friction, G. van der Zwan and J.T. Hynes 152 (1991) 169
Outer-sphere electron-transfer reactions in model molecular solvents: the mean spherical approximation, Y. Zhou, H.L. Friedman and G. Stell 152 (1991) 185
Velocity dependence of friction, S.-B. Zhu, S. Singh, J. Lee and G.W. Robinson 152 (1991) 221
Electron spin exchange in micellized radical pairs. I. ^{13}C low field chemically induced dynamic nuclear polarization (CIDNP) and ^{13}C radio frequency stimulated nuclear polarization (SNP), I.A. Shkrob, V.F. Tarasov and E.G. Bagryanskaya 153 (1991) 427
Electron spin exchange in micellized radical pairs. II. Magnetic field and magnetic isotope effects in multinuclear pairs, I.A. Shkrob, V.F. Tarasov and A.L. Buchachenko 153 (1991) 443
Kinetics of the reactions of intrinsic and phosphorus doped polycrystalline silicon with molecular chlorine, Z.H. Walker and E.A. Ogryzlo 153 (1991) 483
On the solution of the Debye–Smoluchowski equation with a Coulomb potential. III. The case of a Boltzmann initial distribution and a perfectly absorbing sink, S.D. Traytak 154 (1991) 263
Low-temperature chemical reactions. Effect of symmetrically coupled vibrations in collinear exchange reactions, V.A. Benderskii, V.I. Goldanskii and D.E. Makarov 154 (1991) 407

Potential of mean force by constrained molecular dynamics: a sodium chloride ion-pair in water, E. Guàrdia, R. Rey and J.A. Padró 155 (1991) 187
New Monte Carlo simulations of many-particle stochastic dynamics: growth of correlations and local self-ordering during annihilation of like particles, R. Brown and N.A. Efremov 155 (1991) 357
Laser-initiated chain reactions and microexplosions in solid solutions of methylcyclopropane and chlorine, T.J. Tague Jr. and C.A. Wight 156 (1991) 141
Theory of diffusion-influenced fluorescence quenching: dependence of the Stern–Volmer curve on light intensity, S. Lee, M. Yang, K.J. Shin, K.Y. Choo and D. Lee 156 (1991) 339
Dissipative relaxation of a low-energy intermediate electronic state in three-level electron transfer, A.M. Kuznetsov and J. Ulstrup 157 (1991) 25
Activated rate processes in the multidimensional case. Consideration of recrossings in the multidimensional Kramers problem with anisotropic friction, A.M. Berezhkovskii and V.Yu. Zitserman 157 (1991) 141
The effect of pressure on the dynamic quenching by oxygen of the excited singlet state of 9,10-dimethylanthracene in solution, A.D. Scully, H. Yasuda, M. Okamoto and S. Hirayama 157 (1991) 271
Laser-initiated chain reactions and microexplosions in solid solutions of methylcyclopropane and chlorine, Chem. Phys. 156 (1991) 141–148. Erratum, T.J. Tague Jr. and C.A. Wright 157 (1991) 305
Computer simulation of partially diffusion-controlled reactions, M.A. López-Quintela and M.C. Buján-Núñez 157 (1991) 307
Molecular dynamics simulation of superoxide interacting with superoxide dismutase, J. Shen and J.A. McCammon 158 (1991) 191
Quantum simulation of conformation reorganization in the electron transfer reactions of tuna cytochrome c, C. Zheng, J.A. McCammon and P.G. Wolynes 158 (1991) 261
Two-dimensional trajectories of tunneling in the symmetric double-well potential, V.A. Benderskii, V.I. Goldanskii and D.E. Makarov 159 (1992) 29
Site-resolved vibronic spectra of matrix-isolated NBr: comparison with model calculations, K. Seranski, M. Winter and U. Schurath 159 (1992) 247
The dynamics of dressed variables, D.M. Charutz and R.D. Levine 159 (1992) 321
Theory of geminate recombination of radical pairs with instantaneously changing spin Hamiltonian. I. General theory and kinematic approximation, A.B. Doktorov, S.A. Mikhailov and P.A. Purtov 160 (1992) 223
Theory of geminate recombination of radical pairs with instantaneously changing spin-Hamiltonian. II. Method of summation of re-encounter contributions, A.B. Doktorov, S.A. Mikhailov and P.A. Purtov 160 (1992) 239

–photochemical
Trans–cis photoisomerization mechanism of carbocyanines: experimental check of theoretical models, G. Ponterini and F. Momicchioli 151 (1991) 111
Degenerate triplet spin exchange in liquid solution studied by pulse NMR, J. Burri and H. Fischer 151 (1991) 279
Photoisomerization dynamics of diphenylbutadiene in compressed liquid alkanes and in solid environment, Ch. Gehrke, R. Mohrschladt, J. Schroeder, J. Troe and P. Vöhringer 152 (1991) 45
Metal carbonyl photochemistry in organic solvents: femtosecond transient absorption and preliminary resonance Raman spectroscopy, A.G. Joly and K.A. Nelson 152 (1991) 69
A quantum chemical study on the alternative mechanisms of the thermal cis–trans isomerization of streptocyanines, T. Krossner and F. Dietz 153 (1991) 63

Core excitation-induced photodesorption of molecular and fragment ions from CO adsorbates on metal surfaces, R. Treichler, W. Wurth, W. Riedl, P. Feulner and D. Menzel 153 (1991) 259
Picosecond time-resolved absorption and fluorescence in the bacteriorhodopsin photocycle: vibrationally-excited species, D. Blanchard, D.A. Gilmore, T.L. Brack, H. Lemaire, D. Hughes and G.H. Atkinson 154 (1991) 155
Kinetics and magnetic field effect in geminate recombination of triplet radical pairs adsorbed onto porous glass studied by laser flash technique, P.P. Levin, I.V. Katalnikov and V.A. Kuzmin 154 (1991) 449
Spatial dispersion of electron transfer probability, A.I. Burshtein, P.A. Frantsuzov and A.A. Zharikov 155 (1991) 91
Photodissociation of CF_3I at 248 nm: kinetic energy dependence of the recoil anisotropy, P. Felder 155 (1991) 435
The effect of pressure on the dynamic quenching by oxygen of the excited singlet state of 9,10-dimethylanthracene in solution, A.D. Scully, H. Yasuda, M. Okamoto and S. Hirayama 157 (1991) 271
The dynamics of the primary event in rhodopsins revisited, A. Warshel, Z.T. Chu and J.-K. Hwang 158 (1991) 303
Time- and temperature dependence of large-scale conformational transitions in myoglobin, R.D. Young, H. Frauenfelder, J.B. Johnson, D.C. Lamb, G.U. Nienhaus, R. Philipp and R. Scholl 158 (1991) 315
Generalized golden rule approach to the H-transfer problem. II. Application to a photochemical reaction, L. Lavtchieva and Z. Smedarchina 160 (1992) 211

Tunnelling

Optical potentials by the complex coordinate method, N. Rom, N. Lipkin and N. Moiseyev 151 (1991) 199
Solvent dynamical effects in electron transfer: the solvent inertial limit and the predicted influence of quantum effects, G.E. McManis, A. Gochev and M.J. Weaver 152 (1991) 107
A Zeeman level crossing study of the symmetry of the potential hindering the torsional oscillator CH_3, W.T. Sobol, I.G. Cameron and M.M. Pintar 152 (1991) 337
Symmetry breaking in thermally activated NH_4 rotation studied by NMR level crossing spectroscopy, S. Clough, A.J. Horsewill, M.R. Johnson, M.A. Mohammed and T. Newton 152 (1991) 343
Proton transfer dynamics in the hydrogen bond. Inelastic neutron scattering, infrared and Raman spectra of $Na_3H(SO_4)_2$, $K_3H(SO_4)_2$ and $Rb_3H(SO_4)_2$, F. Fillaux, A. Lautié, J. Tomkinson and G.J. Kearley 154 (1991) 135
Low-temperature chemical reactions. Effect of symmetrically coupled vibrations in collinear exchange reactions, V.A. Benderskii, V.I. Goldanskii and D.E. Makarov 154 (1991) 407
The potential of the Na_2 $B\,^1\Pi_u$ state, H. Richter, H. Knöckel and E. Tiemann 157 (1991) 217
Proton-transfer dynamics in the hydrogen bond. Inelastic neutron scattering, infrared and Raman spectra of $KH(CF_3COO)_2$ and $CsH(CF_3COO)_2$, F. Fillaux and J. Tomkinson 158 (1991) 113
Quantum simulation of conformation reorganization in the electron transfer reactions of tuna cytochrome **c**, C. Zheng, J.A. McCammon and P.G. Wolynes 158 (1991) 261
Two-dimensional trajectories of tunneling in the symmetric double-well potential, V.A. Benderskii, V.I. Goldanskii and D.E. Makarov 159 (1992) 29
A semiclassical simulation for tunneling dynamics of malonaldehyde and hydrogenoxalate anion, E. Bosch, M. Moreno and J.M. Lluch 159 (1992) 99
Methyl tunnelling in solid diacetyl, A.M. Alsanoosi and A.J. Horsewill 160 (1992) 25
Generalized golden rule approach to the H-transfer problem. II. Application to a photochemical reaction, L. Lavtchieva and Z. Smedarchina 160 (1992) 211

Electron transfer
A classical study on the vibrational motion of a diatomic molecule in a collisional vibronic excitation, R.F.M. Lobo and A.M.C. Moutinho 151 (1991) 95
The probability of non-adiabatic electron transfer as a function of friction, A.I. Burshtein and A.A. Zharikov 152 (1991) 23
Friction effect on the mechanism of photochemical redox processes in solutions, E.I. Kapinus 152 (1991) 83
Solvent dynamical effects in electron transfer: the solvent inertial limit and the predicted influence of quantum effects, G.E. McManis, A. Gochev and M.J. Weaver 152 (1991) 107
Outer-sphere electron-transfer reactions in model molecular solvents: the mean spherical approximation, Y. Zhou, H.L. Friedman and G. Stell 152 (1991) 185
MRCI potential energy functions for the charge transfer reactions $H^+ + HCl$ $(X^1\Sigma^+) \rightarrow H + HCl^+$ $(X^2\Pi_i, A^2\Sigma^+)$, Th. Glenewinkel-Meyer, Ch. Ottinger, P. Rosmus and H.-J. Werner 152 (1991) 409
Resonant two-photon ionization of phenol in methylene chloride doped solid argon using 248 nm KrF laser and 254 nm Hg lamp radiation, a comparative study. The UV/VIS absorption spectrum of phenol radical cation, K. Kesper, F. Diehl, J.G.G. Simon, H. Specht and A. Schweig 153 (1991) 511
Spatial dispersion of electron transfer probability, A.I. Burshtein, P.A. Frantsuzov and A.A. Zharikov 155 (1991) 91
A cluster model of the charge transfer interaction between an impurity and the host molecular crystal, P. Petelenz and A. Eilmes 155 (1991) 247
Electron transfer induced by liquid defect motion. Exact solution, D.V. Matyushov 155 (1991) 331
Localization and correlation corrections in electronic interactions through single bonded hydrocarbon spacers, M. Braga, A. Broo and S. Larsson 156 (1991) 1
Dissipative relaxation of a low-energy intermediate electronic state in three-level electron transfer, A.M. Kuznetsov and J. Ulstrup 157 (1991) 25
Dynamics of charge transfer chemical reactions in a polar medium within the scope of the Born–Kirkwood–Onsager model, M.V. Basilevsky and G.E. Chudinov 157 (1991) 327
The configuration interaction theory for charge transfer chemical processes in a polar solvent, M.V. Basilevsky and G.E. Chudinov 157 (1991) 345
Radiative and radiationless depopulation of the excited intramolecular charge transfer states: aryl derivatives of aromatic amines, J. Herbich and A. Kapturkiewicz 158 (1991) 143
Quantum simulation of conformation reorganization in the electron transfer reactions of tuna cytochrome c, C. Zheng, J.A. McCammon and P.G. Wolynes 158 (1991) 261
On the photo-sensitized injection of electrons into SnO_2 from cyanine dyes incorporated in Langmuir–Blodgett films, G. Biesmans, M. Van der Auweraer, C. Cathry, F.C. De Schryver, Y. Yonezawa and T. Sato 160 (1992) 97

Positron annihilation
Li-doped MgO as catalysts for oxidative coupling of methane: a positron annihilation study, G.H. Dai, Q.J. Yan, Y. Wang and Q.S. Liu 155 (1991) 275

Ionization (including Rydberg states)
Model studies on femtosecond time-resolved ionization spectroscopy of excited-state vibrational dynamics and vibronic coupling, M. Seel and W. Domcke 151 (1991) 59

Photoionization mass spectrometry of kinetic energy-selected ions. An ion retarding potential difference method applied to NO^+ and O^+ from N_2O, R. Locht, G. Hagenow, K. Hottmann and H. Baumgärtel 151 (1991) 137
The structures and stability of the $Si_3H_6^{2+}$ dications. A theoretical study, T. Kudo and S. Nagase 153 (1991) 379
Highly excited states of nitric oxide studied by high-resolution resonance-enhanced multiphoton ionization spectroscopy, Y. Luo, Y.D. Cheng, H. Ågren, R. Maripuu, W. Seibt, L. Öhlund, P. Ejeklint, B. Carman, K.Z. Xing, Y. Achiba and K. Siegbahn 153 (1991) 473
Absolute partial photoionization cross sections of ethylene, F.A. Grimm, T.A. Whitley, P.R. Keller and J.W. Taylor 154 (1991) 303
The first ionization potentials of some MH_{k+1}^- and $M_2H_{2k+1}^-$ anions calculated by a Green's function method, A.I. Boldyrev and W. von Niessen 155 (1991) 71
Shape resonances in photoionizations of cyanoacetylene. Experimental and theoretical investigations of the $\tilde{X}\,^2\Pi$, $\tilde{A}\,^2\Sigma$ and $\tilde{B}\,^2\Pi$ ionizations up to a photon energy of 28 eV, J. Kreile, H.-D. Kurland, W. Seibel and A. Schweig 155 (1991) 99
Photoionisation and ZEKE photoelectron spectroscopy of Ar, H_2 and CO_2 using a coherent XUV laser source, H.H. Fielding, T.P. Softley and F. Merkt 155 (1991) 257
The photoionization of ammonia revisited. The vibrational autoionization of NH_3 and its three isotopomers in the 10–12 eV photon energy range, R. Locht, B. Leyh, W. Denzer, G. Hagenow and H. Baumgärtel 155 (1991) 407
Total ionization cross sections for $Ne^{**}\{(2p)^5(3p); J=3\}$-molecule systems: absolute values and polarization effects, J.P.J. Driessen, M.P.I. Manders, F.J.M. van de Weijer, G.J. Sandker, W. Boom, H.C.W. Beijerinck and B.J. Verhaar 155 (1991) 447
Localization and correlation corrections in electronic interactions through single bonded hydrocarbon spacers, M. Braga, A. Broo and S. Larsson 156 (1991) 1
Vibronic coupling in Rydberg series of linear molecules, A. Staib, W. Domcke and A.L. Sobolewski 156 (1991) 21
Many-body calculations of the core hole spectra of NiCO, M. Ohno and P. Decleva 156 (1991) 309
Theoretical study of optical excitations of linear C_4^-, L. Adamowicz 156 (1991) 387
Zeeman effect in the two-photon excitation spectrum of the $C^2\Pi$ state of NO, S. Guizard, N. Shafizadeh, D. Chapoulard, M. Horani and D. Gauyacq 156 (1991) 509
Modified version of the trajectory surface leaking method for dynamical calculations on autoionizing atom–diatom collision systems, J. Vojtík and I. Paidarová 157 (1991) 67
The vibrational constant of the $O_2^{2+}X\,^1\Sigma_g^+$ state from the dissociative decay of $n=3,4$ Rydberg states in O_2^+, W.J. van der Zande 157 (1991) 287
The benzene dication: energies of excited states determined by double-charge-transfer spectroscopy using OH^+ and F^+ projectile ions, W.J. Griffiths and F.M. Harris 157 (1991) 299
Many-body calculation of the valence photoemission spectrum of ferrocene, M. Ohno, W. von Niessen and J. Schüle 158 (1991) 1
Rotational distributions of $N_2O^+(\tilde{A}\,^2\Sigma^+)$, $CO_2^+(\tilde{A}\,^2\Pi_u)$ and $CS_2^+(\tilde{A}\,^2\Pi_u)$ produced by electron-impact ionization, I. Tokue, A. Masuda, H. Kume and Y. Ito 158 (1991) 161
Satellite lines at the ionization threshold in charge transfer systems, W. Wardermann and W. von Niessen 159 (1992) 11
Excited states of hydrogen emitted from a graphite diffusion source: Arrhenius behaviour, E. Wallin and L. Holmlid 159 (1992) 313
UV photoemission spectroscopic studies on molecular aggregation of triphenylamines dispersed in polycarbonate thin films, N. Sato and M. Yoshikawa 160 (1992) 289

The electronic structure of poly(*p*-phenylene vinylene), N. Sato, M. Lögdlund, R. Lazzaroni, W.R. Salaneck, J.-L. Brédas, D.D.C. Bradley, R.H. Friend and K.E. Ziemelis 160 (1992) 299
Many-body calculation of the XPS core hole spectra of NiN_2, P. Decleva and M. Ohno 160 (1992) 341
Many-body calculation of the core hole spectra of PdCO, P. Decleva and M. Ohno 160 (1992) 353
Photoionization mass spectrometry of kinetic energy-selected ions. The translational energy distribution of N^+/N_2 in the inner-shell ionization energy range, R. Locht, W. Denzer, E. Rühl and H. Baumgärtel 160 (1992) 477

Molecular motion (including diffusive)

Picosecond photodissociation and geminate radical recombination in alkane solutions of tetraphenylhydrazine, M.G. Hyde and G.S. Beddard 151 (1991) 239
Photoisomerization dynamics of diphenylbutadiene in compressed liquid alkanes and in solid environment, Ch. Gehrke, R. Mohrschladt, J. Schroeder, J. Troe and P. Vöhringer 152 (1991) 45
Nonexponential solvation dynamics of simple liquids and mixtures, W. Jarzeba, G.C. Walker, A.E. Johnson and P.F. Barbara 152 (1991) 57
Solvent cage effects and chemical dynamics in liquids, F. Patron and S.A. Adelman 152 (1991) 121
Ion solvation dynamics in an interaction-site model solvent, F.O. Raineri, Y. Zhou, H.L. Friedman and G. Stell 152 (1991) 201
Velocity dependence of friction, S.-B. Zhu, S. Singh, J. Lee and G.W. Robinson 152 (1991) 221
Anomalous magnetic effects. The role of association in the recombination of singlet radical pairs in liquids, N.V. Shokhirev, E.C. Korolenko, M.B. Taraban and T.V. Leshina 154 (1991) 237
On the solution of the Debye–Smoluchowski equation with a Coulomb potential. III. The case of a Boltzmann initial distribution and a perfectly absorbing sink, S.D. Traytak 154 (1991) 263
Structure and dynamics of polar liquids: a molecular dynamics investigation of N,N-dimethyl formamide, S. Yashonath and C.N.R. Rao 155 (1991) 351
The trans-stilbene–Ar van der Waals complex. Vibrationally averaged substitution structure in its S_0 and S_1 electronic states, B.B. Champagne, D.F. Plusquellic, J.F. Pfanstiel, D.W. Pratt, W.M. van Herpen and W.L. Meerts 156 (1991) 251
Effects of solvent viscoelasticity in the solvation dynamics of an ion in a dense dipolar liquid, A. Chandra and B. Bagchi 156 (1991) 323
Intramolecular dynamics of the C_4H_8NH radical cation. An application of the anisotropic exchange theory for powder ESR lineshapes, L. Sjöqvist, N.P. Benetis, A. Lund and J. Maruani 156 (1991) 457
On the fluorescence depolarization in bis-(N-carbazolyl) compounds, M. Hennecke and H.F. Kauffmann 157 (1991) 391
Photothermal grating spectroscopy study of nongeminate atom recombination of photodissociated iodine in liquids, X.R. Zhu and J.M. Harris 157 (1991) 409
The condensed phases of pyrazine: a test of the Williams–Weller intermolecular potential, Z. Gamba 158 (1991) 59
Pulsed field gradient NMR for the study of the structure of membrane systems, V.A. Daragan and E.E. Ilyina 158 (1991) 105
Diffusion of molecular oxygen in pairs (anthracene–O_2) in glassy matrices, V.V. Korolev, D.G. Sushkov and N.M. Bazhin 158 (1991) 129
Molecular dynamics simulation of superoxide interacting with superoxide dismutase, J. Shen and J.A. McCammon 158 (1991) 191
Comparison of lattice Monte Carlo dynamics and Brownian dynamics folding pathways of α-helical hairpins, A. Rey and J. Skolnick

158 (1991) 199
An NMR study of the backbone dynamics of staphylococcal nuclease in the crystalline state, H.B.R. Cole and D.A. Torchia 158 (1991) 271
The effects of environment and hydration on protein dynamics: a simulation study of myoglobin, P.J. Steinbach, R.J. Loncharich and B.R. Brooks 158 (1991) 383
Theory of long time peptide dynamics: test of various reduced descriptions and role of internal variables, Y. Hu, G.R. Fleming, K.F. Freed and A. Perico 158 (1991) 395
The effects of solvent on the conformation and the collective motions of protein: normal mode analysis and molecular dynamics simulations of melittin in water and in vacuum, A. Kitao, F. Hirata and N. Gō 158 (1991) 447
Dynamics of the hydrate and amide groups of crystalline ribonuclease and lysozyme, M.G. Usha, J. Speyer and R.J. Wittebort 158 (1991) 487
Master equation for site distributions describing barrier crossing in the presence of anisotropic diffusion, G.J. Moro 159 (1992) 421
The structure and dynamics of 1,3,5-cycloheptatriene and 1,3-cycloheptadiene radical cations in low temperature matrices. An ESR investigation, Y. Kubozono, T. Miyamoto, M. Aoyagi, M. Ata, Y. Matsuda, Y. Gondo, H. Nakamura and T. Matsuo 160 (1992) 421

Fluctuations and noise

Three-time autocorrelation function of the power associated with a Gaussian random process, L. Song and J.M. Schurr 155 (1991) 63
Electron transfer induced by liquid defect motion. Exact solution, D.V. Matyushov 155 (1991) 331
Fluorescence and molecular dynamics study of the internal motion of the buried tryptophan in bacteriophage T4 lysozyme: effects of temperature and alteration of nonbonded networks, D.L. Harris and B.S. Hudson 158 (1991) 353

Collective motion and excitations

Nonexponential solvation dynamics of simple liquids and mixtures, W. Jarzeba, G.C. Walker, A.E. Johnson and P.F. Barbara 152 (1991) 57
Hole pairing on oxygen sites in high-T_c copper–oxide superconductors induced by an effective exchange interaction: a theoretical and numerical investigation on planar lattices, A. Ferretti and A. Lami 155 (1991) 179
Molecular dynamics simulation of crystalline imidazole, S. Besnainou, G. Cardini and D.A. Dows 156 (1991) 71
Electronic spectra of 4-nitro-pyridine-*n*-oxide (NPO) single crystals, M. Pierre, P.L. Baldeck, D. Block, R. Georges, H.P. Trommsdorff and J. Zyss 156 (1991) 103
Fluorescence depolarization in nonlinear molecular pairs, D. Gülen 156 (1991) 123
Effects of solvent viscoelasticity in the solvation dynamics of an ion in a dense dipolar liquid, A. Chandra and B. Bagchi 156 (1991) 323
Activated rate processes in the multidimensional case. Consideration of recrossings in the multidimensional Kramers problem with anisotropic friction, A.M. Berezhkovskii and V.Yu. Zitserman 157 (1991) 141
Comparison of lattice Monte Carlo dynamics and Brownian dynamics folding pathways of α-helical hairpins, A. Rey and J. Skolnick 158 (1991) 199

Surface effects and catalysis

Kinetics of the reactions of intrinsic and phosphorus doped polycrystalline silicon with molecular chlorine, Z.H. Walker and E.A. Ogryzlo 153 (1991) 483

Li-doped MgO as catalysts for oxidative coupling of methane: a positron annihilation study, G.H. Dai, Q.J. Yan, Y. Wang and Q.S. Liu 155 (1991) 275
The influence of physisorption and the Eley–Rideal mechanism on a surface reaction: $CO+O_2$, J. Mai and W. von Niessen 156 (1991) 63
A theoretical study of the chemisorption of methane on a Ni(100) surface, O. Swang, K. Faegri Jr., O. Gropen, U. Wahlgren and P. Siegbahn 156 (1991) 379
Lie algebraic approach to scattering of molecules from a solid surface, S. Lin, X. Yi and L. Cai 160 (1992) 163
Nuclear quadrupole interaction of $^{99}Mo(\beta^-)^{99}Tc$ in various molybdenum sulfur cluster compounds and thermal decomposition products of $(NH_4)_2[Mo_3S(S_2)_6]\cdot nH_2O$ ($n=0$–2), P. Mottner, A. Lerf, T. Butz, H. Knözinger, A. Müller, V. Wittneben and E. Krickemeyer 160 (1992) 327
Many-body calculation of the XPS core hole spectra of NiN_2, P. Decleva and M. Ohno 160 (1992) 341
Many-body calculation of the core hole spectra of PdCO, P. Decleva and M. Ohno 160 (1992) 353

Thermodynamic and transport properties
Heavy ions in mixtures of light gases: Fokker–Planck equation and its solution, L. Ferrari 153 (1991) 115
Generalized Einstein relations for ions in molecular gases, A.D. Koutselos and E.A. Mason 153 (1991) 351
The two-dimensional electrolytic solution in the hypernetted chain approximation, W. Chung and S.S. Mak 155 (1991) 19
Potential of mean force by constrained molecular dynamics: a sodium chloride ion-pair in water, E. Guàrdia, R. Rey and J.A. Padró 155 (1991) 187
Monte Carlo and mean field studies of a polyelectrolyte in salt solution, C.E. Woodward and B. Jönsson 155 (1991) 207
Scaling the WCA reference system for two-dimensional Lennard-Jones fluids, F. Cuadros and A. Mulero 156 (1991) 33
Specific heat from an unsymmetrical double well potential, I.D. Feranchuk, A.P. Ulyanenkov and V.S. Kuz'min 157 (1991) 61
Interaction potentials in rare gas–halide ion systems, V. Kellö and A.J. Sadlej 157 (1991) 123
Chemical potential, partial enthalpy and partial volume of mixtures by *NPT* molecular dynamics, D.M. Heyes 159 (1992) 149
A validity test of the WCA perturbation theory for two-dimensional Lennard-Jones fluids, F. Cuadros and A. Mulero 160 (1992) 375

Structure of solids and liquids
Cluster structure in model electrolyte solutions, J.L.F. Abascal and P. Turq 153 (1991) 79
Polyatomic fluids near solid surfaces: a weighted-density-functional approach, T.A. Cherepanova and A.V. Stekolnikov 154 (1991) 41
The two-dimensional electrolytic solution in the hypernetted chain approximation, W. Chung and S.S. Mak 155 (1991) 19
Material properties of low-dimensional charge-transfer salts. I. Charge fluctuations in systems with stronger electronic correlations, M.C. Böhm and A. Staib 155 (1991) 27
Material properties of low-dimensional charge-transfer salts. II. Mode-softening, Peierls transitions and van Hove singularities, M.C. Böhm 155 (1991) 49
Hole pairing on oxygen sites in high-T_c copper–oxide superconductors induced by an effective exchange interaction: a theoretical and numerical investigation on planar lattices, A. Ferretti and A. Lami 155 (1991) 179

On the elastic properties of lithium, sodium and potassium oxide. An ab initio study, R. Dovesi, C. Roetti, C. Freyria-Fava, M. Prencipe and V.R. Saunders 156 (1991) 11
Zinc ion in water: intermolecular potential with approximate three-body correction and Monte Carlo simulation, Y.P. Yongyai, S. Kokpol and B.M. Rode 156 (1991) 403
The condensed phases of pyrazine: a test of the Williams–Weller intermolecular potential, Z. Gamba 158 (1991) 59
Molecular dynamics simulations of water–methanol mixtures, G. Pálinkás, E. Hawlicka and K. Heinzinger 158 (1991) 65
Pulsed field gradient NMR for the study of the structure of membrane systems, V.A. Daragan and E.E. Ilyina 158 (1991) 105
The radial distribution function for two-dimensional Lennard-Jones fluids: computer simulation results, F. Cuadros and A. Mulero 159 (1992) 89
Test of effective pair potential models by molecular dynamics simulation on liquid OCS, J. Samios, H. Stassen and T. Dorfmüller 160 (1992) 33
Nuclear quadrupole interaction of $^{99}Mo(\beta^-)^{99}Tc$ in various molybdenum sulfur cluster compounds and thermal decomposition products of $(NH_4)_2[Mo_3S(S_2)_6]\cdot nH_2O$ (n=0–2), P. Mottner, A. Lerf, T. Butz, H. Knözinger, A. Müller, V. Wittneben and E. Krickemeyer 160 (1992) 327
A validity test of the WCA perturbation theory for two-dimensional Lennard-Jones fluids, F. Cuadros and A. Mulero 160 (1992) 375
Comparative studies of the underlying local order corresponding to different radial distribution functions of disordered materials, G. Tóth and L. Pusztai 160 (1992) 405

Critical phenomena

The influence of physisorption and the Eley–Rideal mechanism on a surface reaction: $CO+O_2$, J. Mai and W. von Niessen 156 (1991) 63
On the critical scattering phenomena of a nonpolar fluid composed of chiral molecules, E.-K. Lee, D.J. Lee and S.K. Kim 157 (1991) 135

Phase transitions

Xerographic discharge of organic thermoplastic material, J.Y. Moisan, B. André, R. Lever and C. Servens 153 (1991) 465
Material properties of low-dimensional charge-transfer salts. I. Charge fluctuations in systems with stronger electronic correlations, M.C. Böhm and A. Staib 155 (1991) 27
Material properties of low-dimensional charge-transfer salts. II. Mode-softening, Peierls transitions and van Hove singularities, M.C. Böhm 155 (1991) 49
Simulation of the unstable dynamics of excitable biomembranes: properties of a cyclic electrochemical gating mechanism, K.D. Schulze 156 (1991) 43
The influence of physisorption and the Eley–Rideal mechanism on a surface reaction: $CO+O_2$, J. Mai and W. von Niessen 156 (1991) 63

Chemically Modified Surfaces

Proceedings of the Fourth Symposium on Chemically Modified Surfaces, Chadds Ford, PA, July 31-August 2, 1991

edited by **H.A. Mottola,** Oklahoma State University, Stillwater, OK, USA and **J.R. Steinmetz,** Hüls America Inc., Bristol, PA, USA

This volume contains the papers presented at the Fourth Symposium on Chemically Modified Surfaces which provided a forum for the presentation of new scientific contributions on chemical modification of different materials, surface characterization, and ancillary topics. Particular attention was paid to the external structure of solids as addressed by fractal considerations, the expanding field of polymer modification, and the chemical modification of membranes and films. Traditional topics in this series of symposia (e.g. different modification of silica surfaces, especially via silane modification and the different analytical techniques to assess the degree and characteristics of the modification) have also received considerable coverage. The book presents the latest developments on surface modification and characterization of polymers, membranes as well as inorganic surfaces.

Contents: Chemical Immobilization in Chemistry *(H.A. Mottola).* Fractal Surfaces: A Dilemma in the Characterization of Porous Glasses *(J.M. Drake et al.).* **Characterization of Chemically Modified Surfaces.** Molecular Transport at Silica/Solution Interfaces *(J.M. Harris et al.).* The Synthesis, Characterization and Modification of Hydride Silica Surfaces *(J.J. Pesek et al.).* Probing Chemically Modified Metal/Polymer Interphases Using Sputtered Neutral Mass Spectrometry *(T.E. Gentle et al.).* A Novel Method for Characterization of Functional Groups on the Surface of Glass *(R. Gnanasekaran et al.).* Solid State NMR Investigations of Saturated and Unsaturated Bonded Phases for High-Performance Liquid Chromatography *(K. Albert et al.).* Inverse Gas Chromatography of Uncoated and Stearate Coated Calcium Carbonate *(J.O. Okonkwo et al.).* **Modification of Polymer Surfaces.** Surface Modification of Polymers *(D.E. Bergbreiter).* Surface vs. Internal Reactivity of Solid Polymers *(W.T. Ford).* Poly(ether ether ketone) Surface Chemistry *(N.L. Franchina et al.).* **Chemical Modification of Silica and Related Studies.** The Fluorination of Silica *(J.H. Clark et al.).* Kinetic Studies of Solution and Gaseous Phase Silylation of Silica Using Variable-Temperature Diffuse Reflectance FTIR Spectroscopy *(K.G. Proctor et al.).* Polymer Encapsulated Stationary Phases *(H. Engelhardt et al.).* Gas Adsorption on Silylated Silica *(H. Barthel).* Anchoring and Reactivity of Ruthenium Tetraammines on Silica and Poly(4-vinylpyridine) *(M.T. Hoffmann et al.).* **Chemical Modification of Membranes and Films.** Immobilization of Amphiphilic Membranes for the Development of Optical and Electrochemical Biosensors *(J.D. Brennan et al.).* Novel Supports for the Development of High Stability Fiber-Optic-Based Immunoprobes *(K.S. Litwiler et al.).* Electrochemical Characterization of Conducting Polymer Containing Molybdenum Sulfide Species *(S. Ye et al.).* Chemical Modification of Dielectric Thin Films for Superconductor Applications *(B. Yarar et al.).* **General Topics on Modification and Characterization of Surfaces.** Modification and Surface Characterization of Talc *(E. Papirer et al.).* Modification of Poly(olefin) Surfaces by Flame Treatment *(E. Papirer et al.).* Kinetics and Mechanism of Low-Temperature Oxygen Uptake by Copper-Containing Carbon Molecular Sieves *(P.K. Sharma).* Abstracts of Unpublished Papers. Author Index.

1992 xiv + 400 pages
US$ 197.00 / Dfl. 345.00
ISBN 0-444-89305-9

Elsevier Science Publishers
P.O. Box 211, 1000 AE Amsterdam, The Netherlands
P.O. Box 882, Madison Square Station, New York, NY 10159, USA

THERMOCHIMICA ACTA

An international journal concerned with the broader aspects of thermochemistry and its applications to chemical problems

Editor-in-Chief:

W.W. Wendlandt, University of Houston, Houston, TX, USA

Thermochimica Acta publishes original research contributions in thermal analysis, thermochemistry, and chemical thermodynamics. Specific areas of research include:

- Static calorimetry of all types
- Dynamic calorimetry of all types including differential scanning calorimetry (DSC), specific heat calorimetry, and others
- Low and high temperature thermodynamic studies of all types
- Thermal analysis techniques of all types such as thermogravimetry (TG), differential thermogravimetry (DTG), differential thermal analysis (DTA), evolved gas detection (or analysis), all types of pyrolysis procedures, high temperature X-ray, nuclear magnetic resonance, infrared and reflectance spectroscopy, electrical conductivity, magnetic and other measurements.

Subscription Information:

1992: Volumes 187-206 (in 40 issues)
Dfl. 5580.00 / US$ 3049.00 (including postage)
ISSN 0040-6031

For a Free Sample Copy Write to:

Elsevier Science Publishers
P.O. Box 330
1000 AH Amsterdam
The Netherlands
Tel: (+31-20) 5862 822
Fax: (+31-20) 5862 845

in the USA & Canada
P.O. Box 882
Madison Square Station
New York, NY 10159, USA
Tel: (212) 633 3750
Fax: (212) 633 3764

ELSEVIER SCIENCE PUBLISHERS

140\j\TCA

Physics of Laser Plasma

edited by **A. Rubenchik**, *Institute of Automation and Electrometry, Novosibirsk, U.S.S.R. and* **S. Witkowski**, *Max-Planck Institut für Quantenoptik, Garching, F.R.G.*

(Handbook of Plasma Physics, Volume 3)

1991 ix + 654 pages
Price: US $ 228.50 / Dfl. 400.00
ISBN 0-444-87426-7

Volume 3 of the Handbook of Plasma Physics continues the trend set by the first two in discussing many of the challenging problems in basic plasma physics. This volume provides a comprehensive review of laser fusion plasma physics and contains the most up-to-date information on high density plasma physics and radiation transport, useful for astrophysicists and high density physicists.

Contents: Editorial preface. Preface to volume 3. 1. Laser plasma and inertial confinement fusion *(C. Yamanaka)*. 2. Atomic physics of laser-produced plasmas *(R.M. More)*. 3. X-ray radiation from laser plasma *(R. Kauffman)*. 4. Laser generated intense thermal radiation *(R. Sigel)*. 5. Direct drive fusion studies *(M.C. Richardson)*. 6. Symmetry and stability physics in laser fusion *(S.E. Bodner)*. 7. Anomalous dissipation of strong electromagnetic waves in a laser plasma *(R.Z. Sagdeev, V.D. Shapiro and V.I. Shevchenko)*. 8. Strong Langmuir turbulence in laser plasma *(A.M. Rubenchik and V.E. Zakharov)*. 9. Laser-plasma interactions *(H.A. Baldis, E.M. Campbell and W.L. Kruer)*. 10. Resonance absorption and ponderomotive action *(P. Mulser)*. 11. Laser accelerators *(F.F. Chen)*. 12. Magnetic fields in laser-produced plasma *(L.A. Bolshov et al.)*. 13. Heat flux inhibition in laser-produced plasma *(A.A. Galeev and A.M. Natanzon)*. 14. Energy transport in laser-produced plasmas *(M.H. Key)*. Author index. Subject index.

Please contact the publisher for detailed information on the Handbook of Plasma Physics, volumes 1 and 2.

NORTH-HOLLAND

Elsevier Science Publishers
P.O. Box 103
1000 AC Amsterdam
The Netherlands

In the USA & Canada:
Elsevier Science Publishing Co., Inc.
P.O. Box 882, Madison Square Station
New York, NY 10159, USA

US $ prices are valid only in the USA and Canada. In all other countries, the Dutch Guilder price is definitive. Customers in The Netherlands, please add 6% BTW. In New York State, applicable sales tax should be added. All prices are subject to change without prior notice.
404/B/500

Handbook on Synchrotron Radiation, Volume 4

Medical, Biological and Physiological Applications

edited by **S. Ebashi, M. Koch** *and* **E. Rubenstein**

1991 xiv + 764 pages Price: US $ 210.00 / Dfl. 410.00 ISBN 0-444-87423-2

The first three volumes in this series were mainly devoted to applications of Synchrotron Radiation in various fields of physics and chemistry. Volume 4 covers in a self-contained manner the properties of sources, elements of instrumentation and applications to biological and medical research. The exception confirming the rule is EXAFS where it was felt that this topic at the border between inorganic chemistry and biochemistry was adequately covered in previous volumes and in several recently published textbooks. Each chapter provides an introduction for newcomers as well as a reference for more advanced researchers. In conclusion this is a unique book providing a comprehensive overview of the use of synchrotron radiation in biology and medicine.

Contents: Preface. 1. Synchrotron X-ray scattering studies of Langmuir films *(J. Als-Nielsen and H. Möwald).* 2. Coronory angiography project at the Photon Factory using a large monochromatic beam *(K. Hyodo, K. Nishimura and M. Ando).* 3. Optical and dielectric properties of materials relevant to biological research *(M.W. Williams, E.T. Arakawa and T. Inagaki).* 4. Crystal-structure analysis of biological macromolecules by synchrotron-radiation diffraction *(H.D. Bartunik).* 5. Fibre diffraction: collagen *(A. Bigi and N. Roveri).* 6. Scattering from non-crystalline systems *(M.H.J. Koch).* 7. Synchrotron radiation sources *(W. Brefeld and P. Gürtler).* 8. A Bragg reflection monochromator for synchrotron radiation angiography *(G.S. Brown).* 9. Trace element analysis by X-ray fluorescence *(A. Iida and Y. Goshi).* 10. Medical applications of synchrotron radiation *(J.C. Giacomini and H.J. Gordon).* 11. Microradiography and microtomography *(W. Graeff and K. Engelke).* 12. NIKOS - non-invasive angiography at HASYLAB *(W. Graeff and W.-R. Dix).* 13. Radiobiological experiments in the X-ray region with synchrotron radiation *(K. Hieda and T. Ito).* 14. Synchrotron radiation for angiography, an overview *(E. Rubenstein and R. Hofstadter).* 15. X-ray microscopy *(G. Schmahl and P.-C. Cheng).* 16. UV-spectroscopy *(E.S. Stevens).* 17. Anomalous X-ray diffraction scattering *(H.B. Stuhrmann, G. Goerigk and B. Munk).* 18. Detectors for angiography *(A. Thompson).* 19. Progress in X-ray synchrotron diffraction studies of muscle contraction *(K. Wakabayashi and Y. Amemiya).* 20A. Imaging apparatus and techniques for synchrotron radiation *(H.D. Zeman).* 20B. The processing of intravenous coronary angiograms produced by synchrotron radiation *(H.D. Zeman).* Author index. Subject index.

NORTH-HOLLAND

Elsevier Science Publishers
P.O. Box 103
1000 AC Amsterdam
The Netherlands

In the USA & Canada:
Elsevier Science Publishing Co., Inc.
P.O. Box 882,
Madison Square Station
New York, NY 10159, USA

US $ prices are valid only in the USA and Canada. In all other countries, the Dutch Guilder price is definitive. Customers in The Netherlands, please add 6% BTW. In New York State, applicable sales tax should be added. All prices are subject to change without prior notice. 415/b/474